```
=> fil wpix
FILE 'WPIX' ENTERED AT 11:51:11 ON 17 DEC 2007
COPYRIGHT (C) 2007 THE THOMSON CORPORATION

FILE LAST UPDATED:                          7 DEC 2007   <20071207/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE:     200779      <200779/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to September
6th
    2007. No update date (UP) has been created for the reclassified
    documents, but they can be identified by 20060101/UPIC and
    20061231/UPIC, 20070601/UPIC and 20071001/UPIC. <<<


FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:
http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
http://scientific.thomson.com/support/patents/coverage/latestupdates/

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:
http://www.stn-international.com/archive/presentations/DWPIAnaVist2_
0710.p
df

 >>> XML document distribution format now available.
                                          See HELP XMLDOC <<<

=>  d his nofile

     (FILE 'HOME' ENTERED AT 10:38:32 ON 17 DEC 2007)

     FILE 'HCAPLUS' ENTERED AT 10:38:41 ON 17 DEC 2007
L1             1 SEA ABB=ON  PLU=ON  US2007026239/PN
                 D SCA

     FILE 'REGISTRY' ENTERED AT 10:39:40 ON 17 DEC 2007
L2            11 SEA ABB=ON  PLU=ON  (108-55-4/BI OR 130973-94-3/BI OR
                 37293-51-9/BI OR 52769-51-4/BI OR 7440-22-4/BI OR
                 9001-54-1/BI OR 9001-63-2/BI OR 9001-78-9/BI OR 9001-92-
7
                 /BI OR 9004-54-0/BI OR 9025-70-1/BI)
                 D SCA

     FILE 'HCAPLUS' ENTERED AT 10:49:06 ON 17 DEC 2007
L3         18567 SEA ABB=ON  PLU=ON  CARBENE?
L4             0 SEA ABB=ON  PLU=ON  L1 AND L3

     FILE 'REGISTRY' ENTERED AT 11:22:31 ON 17 DEC 2007
L5          2747 SEA ABB=ON  PLU=ON  ?DIAZIRIN?/CNS
L6             1 SEA ABB=ON  PLU=ON  L2 AND L5

     FILE 'HCAPLUS' ENTERED AT 11:27:45 ON 17 DEC 2007
L7             QUE ABB=ON  PLU=ON  PHOTOACTIV? OR PHOTOREACTIV? O
                 PHOTOLY? OR PHOTOLINK? OR LIGHTACTIV? OR LIGHTREACTIV?
                 OR LIGHTLINK? OR (LIGHT OR PHOTO)(A)(ACTIV? OR REACTIV?
                 OR LINK?)
```

```
L8            52 SEA ABB=ON  PLU=ON  L5(L)L7
L9               QUE ABB=ON  PLU=ON  (LINK? OR CROSSLINK? OR CROSS(W)
LINK?
                  OR NETWORK?)(2A)(MOLECUL? OR AGENT? OR ADDITIVE? OR
                 COMPOUND? OR COMPD# OR CMPD# OR CPD#) OR LINKER? OR
                 CROSSLINKER?
L10           87 SEA ABB=ON  PLU=ON  L3 AND L9
L11              QUE ABB=ON  PLU=ON  (CHEM? OR COVALENT?)(3A)(ATTACH? OR
                 BIND? OR BOND?)
L12              QUE ABB=ON  PLU=ON  PHOTOCHEM?
L13           73 SEA ABB=ON  PLU=ON  L5(L)L12
L14           11 SEA ABB=ON  PLU=ON  (L8 OR L10 OR L13) AND L11
L15              QUE ABB=ON  PLU=ON  FIBER? OR FABRIC# OR FIBRE? OR
                 FIBRA? OR TEXTILE# OR YARN# OR THREAD? OR NONWOVEN? OR
                 FILAMENT?
L16            3 SEA ABB=ON  PLU=ON  L14 AND L15
L17           11 SEA ABB=ON  PLU=ON  L14 OR L16
                 D AN L16 1-3

     FILE 'WPIX' ENTERED AT 11:41:44 ON 17 DEC 2007
L18          655 SEA ABB=ON  PLU=ON  CARBENE?
                 E US2007026239/PN
L19            1 SEA ABB=ON  PLU=ON  US20070026239/PN
L20              QUE ABB=ON  PLU=ON  ?DIAZIRIN?
L21           76 SEA ABB=ON  PLU=ON  (L18 OR L20) AND L11
L22            1 SEA ABB=ON  PLU=ON  L19 AND L21
                 D KWIC
L23           12 SEA ABB=ON  PLU=ON  L21 AND L9
L24            1 SEA ABB=ON  PLU=ON  L23 AND L15
L25           12 SEA ABB=ON  PLU=ON  L23 OR L24

     FILE 'COMPENDEX' ENTERED AT 11:46:57 ON 17 DEC 2007
L26          371 SEA ABB=ON  PLU=ON  (L18 OR L20) AND L11
L27            8 SEA ABB=ON  PLU=ON  L26 AND L9
L28            0 SEA ABB=ON  PLU=ON  L27 AND L15

     FILE 'JAPIO' ENTERED AT 11:48:32 ON 17 DEC 2007
L29            7 SEA ABB=ON  PLU=ON  (L18 OR L20) AND L11
L30            0 SEA ABB=ON  PLU=ON  L29 AND L9

     FILE 'TEXTILETECH' ENTERED AT 11:49:02 ON 17 DEC 2007
L31            0 SEA ABB=ON  PLU=ON  (L18 OR L20) AND L11

     FILE 'WTEXTILES' ENTERED AT 11:49:20 ON 17 DEC 2007
L32            0 SEA ABB=ON  PLU=ON  (L18 OR L20) AND L11

     FILE 'WPIX' ENTERED AT 11:49:34 ON 17 DEC 2007
                 D AN L19
                 SEL L25 PN,AP

     FILE 'HCAPLUS' ENTERED AT 11:50:07 ON 17 DEC 2007
L33           14 SEA ABB=ON  PLU=ON  (AU2004-206856/AP OR AU2004206856/PN

L34           10 SEA ABB=ON  PLU=ON  L17 NOT L33

     FILE 'HCAPLUS, COMPENDEX' ENTERED AT 11:50:24 ON 17 DEC 2007
L35           18 DUP REM L34 L27 (0 DUPLICATES REMOVED)


=> d l25 ifull 1-12
```

L25 ANSWER 1 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2007-058776 [07] WPIX
DOC. NO. CPI: C2007-021753 [07]
DOC. NO. NON-CPI: N2007-040932 [07]
TITLE: Aqueous coating agent, useful for metallic substrates, comprises a water dispersible- and/or water-soluble polymer with covalently bonded ligands and a polymer with cross-linking functional groups and complementary functional groups
DERWENT CLASS: A82; G02; M13; P42
INVENTOR: DORNBUSCH M
PATENT ASSIGNEE: (BADI-C) BASF COATINGS AG
COUNTRY COUNT: 111

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
DE 102005023728	A1	20061130	(200707)*	DE	12[0]	
WO 2006125498	A1	20061130	(200707)	DE		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 102005023728	A1	DE 2005-102005023728	20050523
WO 2006125498	A1	WO 2006-EP3545	20060419

PRIORITY APPLN. INFO: DE 2005-102005023728 20050523
INT. PATENT CLASSIF.:
IPC ORIGINAL: B05D0007-16 [I,A]; B05D0007-16 [I,C]; C08F0008-00 [I,A]; C08F0008-00 [I,C]; C09D0005-00 [I,A]; C09D0005-00 [I,C]; C09D0005-02 [I,A]; C09D0005-02 [I,C]; C09D0005-08 [I,A]; C09D0005-08 [I,C]; C09D0005-12 [I,A]; C09D0005-12 [I,C]; C23C0022-00 [I,A]; C23C0022-00 [I,C]

BASIC ABSTRACT:
DE 102005023728 A1 UPAB: 20070129
NOVELTY - Aqueous coating agent (A) for metallic substrates comprises a water dispersible- and/or water-soluble polymer with covalently bonded ligands, which releases metal ions on the substrate, and forms corrosion and a chelate on the substrate surface; and a polymer with cross-linkable functional groups and complementary functional groups, where the functional groups and the complementary groups are covalently bonded.
DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for: (1) a method to protect corrosion on the metallic substrate comprising immersing the substrate into a bath containing (A) at 20-90degreesC for 1 second to 15 minutes; and (2) a two-stage process for protecting corrosion of the metallic substrates comprising immersing the substrate into a bath containing corrosion protective agent, which causes a conversion on the substrate surface and immersing the substrate into a bath containing (A) at 20-90degreesC for 1 second to 15 minutes.
USE - (A) is useful for metallic substrates (claimed).
ADVANTAGE - (A) exhibits good corrosion protection. TECHNOLOGY FOCUS:
INORGANIC CHEMISTRY - Preferred Components: The cross-

linker exhibits a covalently bonded ligand. The ligand is urea, amine, amide, imine, imide, pyridine, organosulfur compounds, organo phosphor compounds, organoboron compounds, oxime, acetylacetonate, polyalcohol, phyticacid, acetylene and/or carbene. The polymer and cross-linkable groups of the functional and complementary groups are cross-linked by thermal and/or radiation process. The corrosion protective agent is lanthanide metal as cation; a d-block metal except chromium as cation; a d-block metal except chrome containing metal as anion; and an acid, which undergoes oxidation, except phosphorous and/or acid containing chromium. The substrate after the separation of (A) is thermally treated at 50-200degreesC or by irradiation. The substrate contains metals (20 weight%) of iron, aluminum or zinc.

POLYMERS - Preferred Components: The polymer comprises one or more building blocks of polyester, polyacrylate, polyurethane, polyolefin, polyalcohol, polyvinylether, polyvinylamine or polyalkylenimine.

FILE SEGMENT: CPI; GMPI
MANUAL CODE: CPI: A11-B05A; A11-B05D; A12-B04; G02-A05E; M13-H05

L25 ANSWER 2 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2006-184152 [19] WPIX
DOC. NO. CPI: C2006-061133 [19]
DOC. NO. NON-CPI: N2006-159020 [19]
TITLE: Use of polymeric materials containing transition metal-carbene complexes in organic light-emitting diodes, e.g. for computers, TV, advertising panels, domestic appliances, cars, displays and lighting systems
DERWENT CLASS: A13; A14; A26; A89; E11; E12; L03; U12
INVENTOR: BAETE M; BOLD M; DOETZ F; EGEN M; JOHANNES H; KAHLE K; KOWALSKY W; LENNARTZ C; NORD S; SCHILDKNECHT C; SCHMITT H; THELAKKAT M; WAGENBLAST G; JOHANNES H; SCHMITT H W
PATENT ASSIGNEE: (BADI-C) BASF AG
COUNTRY COUNT: 110

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2006018292	A2	20060223	(200619)*	DE	106[1]	
DE 102004040005	A1	20060223	(200619)	DE		
EP 1784471	A2	20070516	(200734)	DE		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2006018292	A2	WO 2005-EP8913	20050817
DE 102004040005	A1	DE 2004-102004040005	20040818
EP 1784471	A2	EP 2005-782164	20050817
EP 1784471	A2	WO 2005-EP8913	20050817

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1784471	A2 Based on	WO 2006018292 A

PRIORITY APPLN. INFO: DE 2004-102004040005 20040818
INT. PATENT CLASSIF.:
IPC ORIGINAL: C07F0015-00 [I,A]; C07F0015-00 [I,C]; C07F0017-00 [I,C]; C07F0017-02 [I,A]; C08J0003-20 [I,A]; C08K0005-00 [I,C]; C08K0005-56 [I,A]; C09K0011-06 [I,A]; C09K0011-06 [I,C]; H01L0051-05 [I,C]; H01L0051-30 [I,A]; H05B0033-14 [I,A]; H05B0033-14 [I,C]; C07F0015-00 [I,C]; C09K0011-06 [I,C]; H01L0051-05 [I,C]; H05B0033-14 [I,C]

BASIC ABSTRACT:
WO 2006018292 A2 UPAB: 20060320
NOVELTY - Polymeric materials containing transition metal- carbene complexes are used in organic light-emitting diodes.
DETAILED DESCRIPTION - The use of polymeric materials (PMAT) containing polymer(s) (other than poly-(N-vinylcarbazole or polysilane) and transition metal complex(es) of formula (I) in organic light-emitting diodes (OLEDS): M1 = Co, Rh, Ir, Nb, Pd, Pt, Fe, Ru, Os, Cr, Mo, W, Mn, Tc, Re, Cu, Ag or Au;
carben = a neutral or monoanionic, mono-, bi- or tri-dentate carbene ligand (or a bis- or tris-carbene ligand);
L = a mono- or di-anionic (preferably mono-anionic), mono- or bi-dentate ligand;
K = a neutral mono- or bi-dentate ligand; n = at least 1 (the carbene ligands may be the same or different if n is more than 1); m, o = 0, 1 or more (same or different L or K if m or o is more than 1);
(n+m+o) depends on the oxidation state and coordination number of M, on the denticity of the ligands and on the charge on the charged ligands, with the proviso that n is at least 1.
INDEPENDENT CLAIMS are included for: (1) polymeric materials (PMAT) containing polymer(s) as listed below and transition metal complex(es) of formula (IB) (2) a method (M1) for the production of PMAT by mixing polymers with (IB)
(3) a method (M2) for the production of PMAT by reacting functionalised polymers (see below) with a functionalised complex of formula (IIIB) in which the functional groups Q are covalently bonded with K, L or a carbene ligand of formula (II)
(4) light-emitting layers containing PMAT (5) OLEDS containing such emitting layers (6) devices with stationary screens containing such OLEDS, such as those in computers, TV sets, printers, kitchen appliances, advertisement panels, lighting or warning panels, or with mobile screens as in mobile phones, laptops, cars or the destination displays on buses or trains.
Do1, Do2 = donor atoms such as C, P, N, O or S (especially N in the case of Do1).
USE - These polymeric materials are used as emitter substances (claimed). Applications include, especially, organic light-emitting diodes for screens etc. in computers, TV sets, printers, kitchen appliances, advertisement panels, lighting or warning panels, mobile 'phones, laptops, cars or the destination displays on buses or trains.
ADVANTAGE - Polymeric materials containing triplet emitters and showing emission in the blue, red and green ranges; these materials are suitable for use as light-emitting layers in OLEDS and can be applied by coating from solution. TECHNOLOGY FOCUS:

ORGANIC CHEMISTRY - Preferred Complexes: Preferred (IB) are complexes of formula (IBa), (IBb), (IBc) and (IBd):

Z, Z' = CH or N;

R groups = various optionally substituted (hetero) hydrocarbyl groups.

Preferred comonomers (IV) are complexes of formula (IVB).

POLYMERS - Preferred Materials: Mixtures containing complex(es) (I) and polymer(s), or materials containing (I) which is/are covalently bonded with polymer(s).

Preferred polymers comprise poly-p-phenylene-vinylenes, polythiophenes, polyfluorenes, polyfluoranthenes, polyacetylenes, polystyrenes, poly(meth)acrylates and copolymers of these.

Covalent polymer-complex linkages involve direct links such as single bonds, -O-, -S-, -NR-, -CONR-, -N=N-, -CO-, -COO- or -OCO- linking groups, preferably 1-15C alkylene (optionally with one or more CH2 groups replaced by O, S, NR, CONR, CO, COO, OCO, N=N, CH=CH or -Ctriple bondC- and/or optionally substituted with alkyl, aryl, halogen, CN or NO2) or 6-18C arylene (optionally substituted with alkyl, aryl, halogen, CN or NO2 etc.), where:R = H, alkyl or aryl.

These materials (PMAT) may be obtained by mixing (I) with the polymer(s), or by reacting functionalised polymers of formula polymer-(T)p with Q-functionalised transition metal complexes of formula (III) in which the group(s) Q is/are covalently linked with one or more ligands K, a ligand L or a carbene ligand.

Q, T = suitable groups for forming a covalent bond, where Q is attached to L, K or carbene and T is covalently bonded to an end group or central unit of the polymer;

s = 1-3 (if s' is more than 1, Q is preferably attached to the carbene);

p = depends on the mol. weight of the polymer and is selected so that the amount of (I) in the PMAT is 0.5-50 (most preferably 1-20) wt% when the polymer itself is luminescent, or 5-50 (most preferably 15-35) wt% if the polymer itself is not luminescent

Or the PMAT may be obtained by the copolymerisation of suitable monomers with comonomers of formula (IV) in which S is linked to K, L and/or carbene.

S = a copolymerisable group attached to L, K or carbene, preferably to carbene;

s = 1-3

Reactions with (III) or (IV) involve Suzuki coupling, Kumada coupling or Yamamoto coupling reactions.

EXTENSION ABSTRACT:

DEFINITIONS - Preferred Definitions: - Q, T = halogen (Br, I or Cl), alkylsulfonyloxy (e.g. trifluoromethanesulfonyloxy), arylsulfonyloxy (e.g. toluene-sulfonyloxy, boron-containing groups, OH, COOH, acid halide, anhydride or ester, -N?=N+ Hal-, SH, SiR2X or NHR; - R, R = H, alkyl or aryl; - these groups may be linked by a single bond to a ligand, preferably to the carbene, or to the polymer, or attached via a linker -(CR'2)q- (in which one or more CR'2 groups may be replaced by O, S, NR, CONR, CO, COO, OCO, CH=CH or C?=C) or via a 6-18C arylene group (optionally substituted with alkyl, aryl, halogen, CN or NO2 etc.); - R = H,

alkyl or aryl; - q = 1-15; - S = halogen (Br, I, Cl), alkyl- or aryl-sulfonyloxy (see above) or boron-containing groups. EXAMPLE - A ligand of formula (1) was obtained by acetylation of 1,2-phenylenediamine followed by the introduction of phenyl groups using a copper catalyst as described in Synthetic Comm., 2000, 30, 3651, and ring closure by reaction with triethyl orthoformate in presence of ammonium tetrafluoroborate. A solution of 1.32 g (1) in 25 ml toluene was treated over 30 minutes with 7.5 ml potassium bis-trimethylsilylamide (0.5-M in toluene), stirred for 30 minutes at room temperature (RT), treated with a solution of 310 mg iridium complex ((mu-Cl)(eta4-1,5-cod)Ir)2 in 30 ml toluene, stirred for 1 hour at RT, 2 hours at 70degreesC and then overnight under reflux, and worked up by filtration, evaporation to dryness and chromatography, to give 0.75 g (82%) of a complex of formula (2) as a fac/mer isomer mixture (characterised by NMR, MS, UV/VIS, DTA and elemental analysis). The mixture (0.46 g) was separated by chromatography on silica gel, to give 0.2886 g pure fac-isomer and 0.0364 g mer-isomer. (Structures (1) and (2), page 79) Tests were carried out with an OLED in which the emitter layer (thickness 61 nm) was made from a 28% solution of (2) in a 2% solution of polymethyl methacrylate in chlorobenzene. This device showed an emission peak at 453 nm, a photometric efficiency of 0.8 cd/A, an external quantum yield of 1% and a luminance of 30 cd/m2. Corresponding values for an OLED with the pure fac-isomer in the emitter layer (30% solution; thickness 27 nm) were 400 nm, 0.53 cd/A, 1.5% and 80 cd/m2.

FILE SEGMENT: CPI; EPI
MANUAL CODE: CPI: A12-E11A; A12-L03; E05-L02A; E05-L02B; E05-L03A; E05-L03B; E05-M02; E05-M03A; E05-M03B; E05-M03C; E05-N02; E05-N03A; E05-N03B; L04-E03A
EPI: U12-A01A1E

L25 ANSWER 3 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2005-796649 [81] WPIX
DOC. NO. CPI: C2005-245414 [81]
TITLE: Use of phosphonium salt derivatives as solubility controlling auxiliaries and as solubility controlling fragments of a molecule or a substrate
DERWENT CLASS: A17; B04; E19; J04
INVENTOR: BOEZIO A; CHARETTE A; POUPON J; POUPON J C
PATENT ASSIGNEE: (VALO-N) VALORISATION RECH SC; (VALO-N) VALORISATION RECH
COUNTRY COUNT: 109

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2005097812	A1	20051020	(200581)*	EN	101[0]	
EP 1756128	A1	20070228	(200718)	EN		
AU 2005231870	A1	20051020	(200724)	EN		
US 20070197477	A1	20070823	(200757)	EN		
BR 2005009757	A	20071016	(200777)	PT		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2005097812	A1	WO 2005-CA523	20050406
US 20070197477	A1 Provisional	US 2004-560592P	20040409

AU 2005231870 A1	AU 2005-231870 20050406
EP 1756128 A1	EP 2005-732193 20050406
EP 1756128 A1	WO 2005-CA523 20050406
US 20070197477 A1 CIP of	WO 2005-CA523 20050406
US 20070197477 A1	US 2006-539075 20061005
BR 2005009757 A	BR 2005-9757 20050406
BR 2005009757 A	WO 2005-CA523 20050406

FILING DETAILS:

PATENT NO	KIND		PATENT NO	
EP 1756128	A1	Based on	WO 2005097812	A
AU 2005231870	A1	Based on	WO 2005097812	A
BR 2005009757	A	Based on	WO 2005097812	A

PRIORITY APPLN. INFO: US 2004-560592P 20040409
WO 2005-CA523 20050406
US 2006-539075 20061005

INT. PATENT CLASSIF.:

IPC ORIGINAL: A61K0031-675 [I,A]; A61K0031-675 [I,C]; C07B0063-00 [I,C]; C07B0063-00 [I,C]; C07B0063-04 [I,A]; C07B0063-04 [I,A]; C07F0009-00 [I,C]; C07F0009-00 [I,C]; C07F0009-54 [I,A]; C07F0009-54 [I,A]; C07K0001-00 [I,C]; C07K0001-00 [I,C]; C07K0001-04 [I,A]; C08F0004-00 [I,C]; C08F0004-00 [I,C]; C08F0004-02 [I,A]; C08K0005-00 [I,C]; C08K0005-50 [I,A]; C07B0063-00 [I,C]; C07B0063-04 [I,A]; C07F0009-00 [I,C]; C07F0009-54 [I,A]; C07K0001-00 [I,C]; C07K0001-04 [I,A]; C08F0004-00 [I,C]; C08F0004-02 [I,A]; C08K0005-00 [I,C]; C08K0005-50 [I,A]

IPC RECLASSIF.: C07B0061-00 [I,A]; C07B0061-00 [I,C]; C07B0063-00 [I,C]; C07B0063-04 [I,A]; C07F0009-00 [I,C]; C07F0009-54 [I,A]; C07F0009-58 [I,A]; C07F0009-59 [I,A]; C07K0001-00 [I,C]; C07K0001-04 [I,A]; C08F0004-00 [I,C]; C08F0004-02 [I,A]; C08K0005-00 [I,C]; C08K0005-50 [I,A]

BASIC ABSTRACT:

WO 2005097812 A1 UPAB: 20060125

NOVELTY - Using phosphonium salt derivatives as solubility controlling auxiliaries and as solubility controlling fragments of a molecule or a substrate, is new.

DETAILED DESCRIPTION - Using phosphonium salt derivatives of formula (I), (II) or (IA) as solubility controlling auxiliaries and as solubility controlling fragments of a molecule or a substrate, is new.

R1-A-P(A-R1)2 (I)

R1-A+-P(A-R1)2-L1 (X-) (II) A'-P(A') (IA).

The molecule is attached to the phosphorous atom of (I) or to a linker attached to the phosphorous atom. (I) is attached to the rest of the molecule by phosphorous atom and (II) is attached to the rest of the molecule by the linker.

A=furyl, phenyl, pyridyl, naphthyl or thiophenyl; R1=T2;

T2=H, halo, OH, OMe, SMe, SPh, SH, 1-6C alkoxy, 1-8C alkyl, 2-8C alkenyl, 2-8C alkynyl, 1-6C aminoalkyl, 6-20C aralkyl, 6-12C aryl, 3-8C cycloalkyl, 1-12C heteroaryl, 1-12C heterocyclyl or 1-6C hydroxyalkyl;

L1=linker;

X-=T1;
T1=F-, Cl-, Br-, I-, ClO4-, PF6-, N3-, BF4-, SbF6-, BH4-, organic acid, acetate or amino acid carboxylate; A'=furyl, phenyl, pyridyl, naphthyl or thiophenyl (optionally mono- - tri-substituted with T2. INDEPENDENT CLAIMS are alos included for: (1) carrying out (m1) a chemical reaction, comprising: (a) attaching a substrate on (I), where the substrate is attached to the phosphorous atom or to a linker attached to the phosphorous atom, chemically modifying the substrate and cleaving the substrate from (I); or (b) solubilizing (I) in a first solvent (1) to obtain a solution, chemically modifying the substrate, adding a second solvent (2) to the solution to cause (I) to precipitate, and separating the precipitate from the solution by filtration, to isolate (I);
(2) carrying out (m2) a chemical reaction, comprising: (a) solubilizing a compound of formula (IIIb) in to obtain a solution; (b) modifying the substrate, to obtain a compound of formula (IV); (c) adding to the solution to precipitate (IV); and (d) separating the precipitate from the solution by filtration to isolate (IV);
(3) compounds (C1) of formula (XX), (XXI), (XXII), (XXIII) or (XXIV);
(4) compounds (C2) of formula (XI), (XII), (XIII), (XXV), (XXVI), (XXVII) or (XVIII);
(5) use of (C1) and (C2) as reagents in a chemical reaction; and
(6) separating two different compounds ((C1) or (C2) or their derivatives) from one another, comprising: (a) selecting a solvent or its mixture to selectively precipitate one compound with respect to the other; and (b) mixing the compounds with the solvent to precipitate one of the compound.
A'+-P(A')2-Z-L2'-R2' (X1-) (XXV) A'+-P(A')(Z-L2'-R2')2 (X1-) (XXVI) A'+-P(A')2-(CH2)n-L2'-R2 (X1-) (XXVII) A'+-P(Z-L2'-R2')3 (X1-) (XXVIII) R1-A+-P(AR1)2-L2-sustrate (X-) (IIIb) R1-A+-P(AR1)2-L2-modified substrate (X-) (IV) R1-A+-P(A-R1)2-Z-L2-R2 (X'-) (XX) R1-A+-P(A-R1)(Z-L2-R2)-Z-L2-R2 (X'-) (XXI) R1-A+-P(A-R1)2-(CH2)n-L2-R2 (X'-) (XXII) R1-A+-P(Z-L2-R2)3 (X'-) (XXIII) R2-L2-Z+-P(Z-L2-R2)3 (X'-) (XXIV) R2=Br, N3, OH, CH2OH, COOH, CHO, C=CH2, linking moiety or a chemical reagent (preferably ruthenium catalyst for olefin metathesis reactions, -C=Ru(T)2P(R5)3, a group of formula (ia) - (if) or oxidizing reagent of formula (ig) or (ih)); L2=linker or a chemical bond; n=0 - 6;
R5=cyclohexyl;
R6=1-6C alkyl or 5-6C cycloalkyl; T=Br, Cl, I or OTf;
r,n=0 - 6;
X'=T1;
X1-=T1, RuO4-, or N(SO2CF3)2-; R10=T2;
R2'=Br, N3, OH, CH2OH, COOH, CHO, N=C=O, C=CH2, linking moiety or a chemical reagent;
L2'=linker or a chemical bond.
USE - As solubility controlling auxiliaries and as solubility controlling fragments of a molecule or a substrate; and in carrying out chemical reactions (Claimed).
ADVANTAGE - By using the phosphonium salt derivatives it is possible to provide a simple support, which has a good loading capacity. The salts over come the major drawbacks of the soluble supports of the prior art.
TECHNOLOGY FOCUS:
ORGANIC CHEMISTRY - Preferred Components: The molecule is an organic reagent (preferably amine reagent, catalyst, ligand, chiral

ligand, linker, coupling reagent, organic substrate, phosphine reagent, tin reagent, silicon reagent or a scavenger). The molecule has a molecular weight of 40 - 1200 (preferably 50 - 1000, especially 60 - 700) g/mol or 40 - 3000 (preferably 50 - 2000, especially 60 - 1400) g/mol. The substrate and (C1) have a molecular weight of 40 - 1200 (preferably 50 - 1000, especially 60 - 700) g/mol. (I) is of formula R1-A+-P(AR1)2-L2-molecule (X-) (IIIa). (IIIa) and the molecule is soluble in (1). (C1) is soluble in (1) and precipitates in a mixture of (1) and (2). (1) is selected from dichloromethane, 1,2-dichloromethane, chloroform, acetonitrile, dimethylformamide, dimethylsulfoxide, benzonitrile or nitrobenzene. (IIIa) and the molecule precipitate in (1) and (2). (2) is selected from diethyl ether, tetrahydrofuran, hexane, toluene, benzene, chlorobenzene, tetrachloromethane and tert-butyl methyl ether. The molecule precipitates by adding (2) to a solution comprising the molecule solubilized in (1).

Preferred Methods: The method (m1) additionally involves cleaving the substrate and recovering the substrate and (I) followed by separate isolation and purification. The method (m2) additionally involves cleaving the modified substrate from the phosphorous atom or from the linker and recovering the modified substrate, followed by its isolation and purification; and recovering (II).

EXTENSION ABSTRACT:

DEFINITIONS - Preferred Definitions: - A=phenyl; - R1=H; - R2 =chemical reagent selected from pyridine, 1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine (substituted at one position), phosphine reagent of formula -P(R7)2 or -P(O)(R7)2, tin reagent of formula -Sn(R8)2T2, -SN(R8)2-CH2-C=C or -Sn(R8)2-C=C, coupling reagent of formula -N=C=NR9 or -NH-C(O)-NH-R9, bipyridine, bis (quinoline), oxazoline, bis(oxazoline), phosphine, N-heterocyclic carbene, substituted binaphthol, 1,2-diol, 1,3-diol, 1,4-diol, aldehyde, tertiary amine, sulfonic acid, or a linking moiety selected from -(CH2)r-OH-C(O)H, -COOH, substituted benzaldehyde, substituted benzoic acid, biphenyl (substituted at 4-position by K1), 3-phenoxy-benzene or phenyl (both substituted at 1-position by K1), 4-acetyl-4-hydroxymethyl-3-nitrophenol-1-yl, 4-hydroxymethyl-3-nitrophenol-1-yl or 4-hydroxymethyl-3-methoxyphenol-1-yl or silicon reagent of formula -Si(R11)(R12)-Cl; - K1=C(CH2)rOH; - R7=methyl or phenyl; - T2=H, Br, Cl or OTf; - R8 =n-butyl; - R9=6C cycloalkyl; - L2=-(CH2)m-, phenyl, biphenyl (optionally substituted at 4-position by -(CH2)q-), -Ph-O-Ph- or -Ph-(CH2)q-Ph-; - m=1 - 8; - q=r; - X'=ClO4 or PF6; - R11,R12 =methyl, ethyl, isopropyl, tert-butyl or phenyl; - R10=-OH or -OMe.

EXAMPLE - Menthol (156 mg) and (3- diphenylphosphinophenyl) triphenyl phosphonium perchlorate (phosphonium salt derivative) (1 g) were dissolved in CH2Cl2 (5 ml). Toluene (10 ml) was then added and the solution was cooled to -5degreesC. Diethylazodicarboxylate (225 mul) was added dropwise over 5 minutes. Then 4-nitrobenzoic acid (220 mg) was added and the solution was warmed slowly to room temperature over 3 hours. After nine hours of stirring at room temperature, Et2O (25 ml) was added to the solution and the resulting solution was worked up to form 4-nitro-benzoic acid (1S,2S,5R)-2-isopropyl-5-methyl-cyclohexyl ester.

FILE SEGMENT: CPI

MANUAL CODE: CPI: A02-A00A; A04-G01A; A10-D03; B05-A02;

B05-A03B; B05-B01B; B05-B01E; B05-B01F; B11-B; B11-C01; B11-C09; E05-E01B; E05-E01C; E05-G01; E05-G02; E11-K; E31-M; E35-X; J04-X

L25 ANSWER 4 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2005-214263 [22] WPIX
DOC. NO. CPI: C2005-068447 [22]
TITLE: Functionalization of yarn or textile product useful in dyeing of fabrics and cloths involves contacting it with linker molecule containing activatable chemical group and functional groups in presence of non-linker molecule
DERWENT CLASS: A87; A96; D16; D22; F06; P73
INVENTOR: BRUININK A; CHAI GAO H; CREVOISIER F; RASCHLE P; SIGRIST H; BILLIA M F; CHAI G H
PATENT ASSIGNEE: (CSEM-N) CSEM CENT SUISSE ELECTRONIQUE & MICROTEC
COUNTRY COUNT: 107

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2005019518	A1	20050303	(200522)*	EN	41[4]	
EP 1664416	A1	20060607	(200638)	EN		
US 20070026239	A1	20070201	(200712)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2005019518	A1	WO 2004-IB2962	20040826
EP 1664416	A1	EP 2004-769354	20040826
EP 1664416	A1	WO 2004-IB2962	20040826
US 20070026239	A1	WO 2004-IB2962	20040826
US 20070026239	A1	US 2006-569510	20060724

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1664416	A1 Based on	WO 2005019518 A

PRIORITY APPLN. INFO: GB 2003-19929 20030826
INT. PATENT CLASSIF.:
IPC ORIGINAL: D06M0010-00 [I,A]; D06M0010-02 [I,A]; D06M0015-03 [I,A]; D06M0015-15 [I,A]; B32B0017-06 [I,A]; B32B0017-06 [I,C]
IPC RECLASSIF.: D06M0010-00 [I,A]; D06M0010-00 [I,C]; D06M0010-02 [I,A]; D06M0015-01 [I,C]; D06M0015-03 [I,A]; D06M0015-15 [I,A]

BASIC ABSTRACT:
WO 2005019518 A1 UPAB: 20050708
NOVELTY - Functionalizing yarn or textile product (A1) comprising contacting a linker molecule containing at least one activatable chemical group and functional groups with (A1), optionally in presence of non- linker molecule; activating the chemical groups to cause covalent attachment of the linker molecule to (A1) and

the non- linker molecule, and providing (A1) with the property of the non-linker molecule, is new.

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for a composition comprising (A1), linker molecule and optionally a non-linker molecule.

USE - The method is useful for functionalizing yarn or textile product (claimed) useful in dyeing of fabrics and cloths; for immobilization to yarn or textile of biomolecules, which are useful in medicines for treating wounds.

ADVANTAGE - The yarn or textile product are obtained with the improved desired property. The linker molecule minimizes the denaturation of biomolecule. The method effectively immobilizes biomolecules on the yarn and textile products, which allows the biomolecules to retain their biological activity. The method allows unrestricted covalent attachment of low and high molecular weight substances to yarns and textiles; and provides controlled release of immobilized species from functionalized yarns and textile products with antibiotic properties. In comparison with current direct chemical derivatization of yarns and textile products by batch processing, linker polymers with activatable chemical reactivity can add beneficial physical and chemical characteristic to a textile. Modification of yarn and textile using linker polymers allows the surface charge and/or surface polarity of the yarn or textile to be changed, and allows the possibility of secondary chemical modification of the yarn or textile. Use of linker polymers allows attachment of dyes, polymers, biomolecules, or inorganic materials to textile of any shape and dimension at any stage in manufacture of the textile.

TECHNOLOGY FOCUS:

TEXTILES AND PAPER - Preferred Method: The non-linker molecule is covalently attached to (A1) in a single reaction step. The linker molecule is contacted with (A1) before the non-linker molecule. The method further involves contacting (A1) with positively charged metal ions (preferably sliver ions) to bind the metal ions to the functional groups before the linker molecule. (A1) is pre-treated with oxygen plasma to improve its wetting properties.

Preferred Components: The linker molecule is multiply substituted with activatable chemical groups. The activatable chemical group (preferably thermochemically or photochemically activatable) is activated with actinic energy and converts to a highly reactive intermediate (preferably carbene intermediate). The linker molecule comprises a natural or synthetic polymer (preferably biopolymer, especially protein, peptide, polysaccharide or dextran-based polymer, especially a polysaccharide and at least two activatable chemical groups). The linker molecule comprises a cleavage site, which is cleaved under predetermined conditions to release the non-linker molecule or functional group from (A1), (preferably a target for hydrolytic enzyme to allow enzyme-induced or biosystem-induced release of the non-linker molecule or functional group, especially a substrate for endoglycosidase or endopeptidase). The linker molecule is either a dextran-based biopolymer comprising a target for dextranase; a hyaluronic acid-based biopolymer

comprising a target for hyaluronidase; a protein-based polymer comprising a target for protease; or a peptide-based polymer comprising a target for endopeptidase. (A1) Is of natural or synthetic origin, a blend of synthetic yarns or a blend of natural and synthetic yarns (preferably synthetic polyester). The functional groups have desired property different from the property of non-linker molecule.

ORGANIC CHEMISTRY - Preferred Components: The non-linker molecule is a solvent, synthetic or natural chemical, synthetic or natural dye, synthetic polymer, a biopolymer, a biomolecule, a biologically active molecule, a synthetic or natural vitamin and/or hormone. The functional group is a positively charged group at neutral pH (such an amino group), negatively charged group at neutral pH (such as carboxyl group), thiol group, or dye such as fluorescent dye (preferably negatively charged group).

BIOLOGY - Preferred Components: The non-linker molecule is preferably enzyme (e.g. lysozyme), a growth factor, an anti-microbial agent, an antibiotic, a fungicide and/or an agent capable of suppressing the proliferation of bacteria or fungi.

EXTENSION ABSTRACT:

EXAMPLE - A polyester tissue was incubated with aqueous solution containing OptoDex A (RTM; linker polymer having photoactive chemical species and amino function) after oxygen plasma treatment and exposed to light for photoimmobilization. After photoimmobilization, the excess OptoDex (RTM; linker polymer having photoactive chemical species and amino function) was removed. Treatment of textile with linker polymer provided improved wetting properties and does not alter the appearance and texture of the sample.

FILE SEGMENT: CPI; GMPI
MANUAL CODE: CPI: A08-M01A; A12-G; A12-S05N; A12-S05P; A12-V01; A12-V03A; A12-W11L; D05-A01A1; D05-A01A2; D05-A01B; D05-H10; D09-C04B; F03-C02; F03-C06; F03-F07; F04-E04

L25 ANSWER 5 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2004-676936 [66] WPIX
DOC. NO. CPI: C2004-241162 [66]
TITLE: Copolymeric hydrogel precursor useful in hydrogel layer for applying to substrate e.g. sensor comprises first monomeric subunits having photocrosslinkable functionality and second monomeric subunits having chemically selective functionality
DERWENT CLASS: A14; A96; B04; B07; D16; D22; G02; P32
INVENTOR: AGROSKIN Y; BOSCHETTI E; HUANG W
PATENT ASSIGNEE: (CIPH-N) CIPHERGEN BIOSYSTEMS INC
COUNTRY COUNT: 106

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2004076511	A2	20040910	(200466)*	EN	259[27]	
US 20070082019	A1	20070412	(200726)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2004076511 A2		WO 2004-US4847	20040220
US 20070082019 A1	Provisional	US 2003-448467P	20030221
US 20070082019 A1		WO 2004-US4847	20040220
US 20070082019 A1		US 2006-546173	20061024

PRIORITY APPLN. INFO: US 2003-448467P 20030221
US 2006-546173 20061024

INT. PATENT CLASSIF.:

IPC ORIGINAL: A61F0002-02 [I,A]; A61F0002-02 [I,C]; C12M0001-34 [I,A]; C12M0001-34 [I,C]

IPC RECLASSIF.: A61L0027-00 [I,A]; A61L0027-00 [I,C]; C08F0290-00 [I,A]; C08F0290-00 [I,C]; C08G [I,S]; C08J0007-00 [I,C]; C08J0007-16 [I,A]; G01N0033-543 [I,A]; G01N0033-543 [I,C]

BASIC ABSTRACT:

WO 2004076511 A2 UPAB: 20051110

NOVELTY - A copolymeric hydrogel precursor (c1) comprising first monomeric subunits (a1) that comprise a photocross-linkable functionality and second monomeric subunits (a2) that comprise a chemically selective functionality for binding a protein, biopolymer or for interacting with a biopolymer, is new.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for the following:

(1) a copolymeric hydrogel prepared (M1) by photocross-linking of (c1);

(2) preparation of (c1), comprising copolymerization of monomeric subunits comprising first monomeric subunits that comprise a first free radical copolymerization functionality and a photocrosslinkable functionality and second monomeric subunits that comprise a second free radical copolymerization functionality and a chemically selective functionality for binding a protein;

(3) a polymeric hydrogel precursor (c2) comprising photocrosslinkable functionality and chemically selective functionality, (c2) is prepared by functionalizing a prefunctionalized polymeric hydrogel precursor with photocrosslinkable functionality and with chemically selective functionality (where the amounts of photocross-linkable functionality and chemically selective functionality provide the hydrogel precursor with the ability to be photocross-linked into the hydrogel and the ability for the hydrogel to be selectively reactive with protein under aqueous conditions, thus the protein becomes bound to the chemically selective functionality); (4) a photocross-linkable hydrogel precursor composition for selective interaction with protein under aqueous conditions contains at least one hydrogel precursor polymer consisting of (a1) and (a2) for interaction with a biomolecular analyte (where the photocross-linkable hydrogel precursor composition is free of photoinitiator);

(5) functionalizing (M2) a surface with copolymeric hydrogel, comprising:

(a) providing a substrate presenting a surface and a copolymeric hydrogel precursor that comprise a photocross-linkable functionality (a3) and second comonomeric subunits that comprise a chemically selective functionality (a4) for binding a molecular analyte;

(b) contacting the copolymeric hydrogel precursor and the surface

to form a layer of the copolymeric hydrogel precursor on the surface; and
(c) photocross-linking at least some of the copolymeric hydrogel precursor layer to form hydrogel in contact with the surface;
(6) a substrate (S1) comprises a substrate surface and a hydrogel on its surface (where the hydrogel comprises a photocross-linked functionality and a chemically selective functionality for binding a biomolecular analyte and is hydrogel is free of photoinitiator, and the amount of the chemically selective functionality is sufficient for binding the biomolecular analyte);
(7) detecting an analyte (M3), comprising: (a) contacting (S1) with a sample (preferably blood sample such as serum sample) that contains a biomolecular analyte; and (b) detecting the biomolecular analyte by virtue of its binding the chemically selective functionality; (8) a particle comprising the copolymeric hydrogel; and (9) a copolymeric hydrogel precursor (c3) comprising a first monomeric subunits that comprise a photocross-linkable functionality and third monomeric subunits that comprise an energy absorbing moiety.

USE - For functionalizing a surface with copolymeric hydrogel; in substrate; for detecting an analyte (all claimed); in hydrogel layer for applying to substrate e.g. sensor, tissue adhesive, drug delivery, dressing, and surface coatings which are used in biomedical devices such as catheters, catheter balloons, and stents as a probe for mass spectroscopy.

ADVANTAGE - The amounts of (a1) and (a2) provide the copolymeric hydrogel precursor with the ability to be photocross-linked into a hydrogel and the ability for the hydrogel to be selectively reactive with protein or biopolymer under aqueous conditions, thus the protein or the biopolymer, becomes bound or adsorbed to the chemically selective functionality. While preparing copolymeric hydrogel precursor, amounts of first and second monomeric subunits provides, upon copolymerization, the polymeric hydrogel precursor with the ability to be photocross-linked into the hydrogel and the ability to be selectively reactive with protein under aqueous conditions, thus protein becomes bound to the chemically selective functionality. (c1) improves Matrix-Assisted Laser Desorption/Ionization (MALDI), Surface-Enhanced Laser Desorption/Ionization (SELDI), and other mass-spectrometric analyses; maximizing the value of a hydrogel surface for SELDI and MALDI analysis including the following factors: complete coverage of the hydrogel, control of hydrogel thickness and swelling degree, uniformity of hydrogel coatings, stability of hydrogel on the surface, controlling the density of the chemically selective, binding functionality, ease and consistency of producing hydrogel, and absence of low molecular weight components which can diffuse out and interfere with the analyses by generating signal noise. (c1) provides better analyses, including laser desorption/ionization mass spectrometry analyses, can be achieved over more diverse systems; provides mild conditions, minimum side-product formation, fast cure times, and spatial control of the cross-linking reaction. Also, the physiochemical properties of the polymer network such as swelling can be modulated by adjusting illumination and concentration of the photocross-linkable group. (c1) provides improved surface area, resulting in increased binding capacity along with marked improvement in binding selectivity; improved control of the cross-linking reaction, thus resulting in a more uniform hydrogel with desired pore size suitable for capturing proteins and biomolecules in a broad range of molecular weight; uses polymerization process to produce polymers which is more consistent and controllable, and use of polymers instead of monomers which provide sufficient viscosity is more compatible with established processing methods and improves chip

manufacturing; produces polymers in bulk allows one to form uniform and consistent coating surface eliminating variations, both, spot-to-spot and chip-to-chip in material composition and film thickness; better and more complete coverage of the hydrogel surface reducing non-specific binding which can affect capturing of analytes and generate signal noise in the mass analysis step; hydrogel materials having greater structural stability, resulting in improved duration life time and consistent sample capturing. As the pore size can be tailored to meet the specific demands of the analyte, the hydrogels can be constructed to be capable of selectively captures hydrogels that can be constructed to be capable of binding proteins having a wide rang of molecular weight.

TECHNOLOGY FOCUS:

POLYMERS - Preferred Components: (c1) is a water-soluble or water-swellable copolymer that upon co-polymerization comprises a linear, carbon backbone (preferably water soluble). (c1) consists of a linear copolymeric backbone having side groups that comprise the photocross-linkable functionality and the chemically selective functionality. In (c2), the prefunctionalized polymeric hydrogel precursor is a hydroxyl functional polymer or is an acrylate, acrylamide, methacrylamide, vinyl polymer, or polysaccharide. In (M2), the polymeric hydrogel precursor that is cross-linked is a uniform layer on the substrate surface and has an average layer thickness of 5 nm-10 microm, the polymeric hydrogel precursor comprises a linear polymeric backbone that is comprised of carbon and that carries first side groups having the photocross-linkable functionality and second side groups having the chemically selective functionality. In (M2), the hydrogel precursor is cross-linked and comprises a cross-linked form of a linear polymeric backbone that has side groups comprising the chemically selective functionality, (where the chemically selective functionality covalently or electrostatically binds protein). In (S1), the hydrogel is a uniform layer (preferably having a thickness of 10 nm-10 microm, especially at most2 microm); in the form of a discreet spots (preferably having a spot thickness of 10 nm-10 microm); is covalently bound to the substrate surface; comprises photocross-linked benzophenone functionality; and is covalently bound to the surface. In (S1), the hydrogel is a uniform layer on the substrate surface having an average layer thickness of 5 nm-10 microm. In (S1), the hydrogel is a copolymeric hydrogel, dextran derivative, or its derivative of poly (2-hydroxyethyl methacrylate) or its copolymer; comprises photocross-linked benzophenone, diazo ester, aryl azide, or diazirine functionality; is a water-swellable polymer that comprises a linear, carbon backbone that has been cross-linked; is a copolymer prepared by cross-linking of a precursor copolymer comprised of carboxylic acid-containing side groups and benzophenone-containing side groups or is free of photoinitiator. In (S1), the chemically selective functionality is an electrophilic or nucleophilic group; an anionic or a cationic group (preferably carboxylic acid, amino, or quaternary amino group).

Preferred Precursor: (c1) is a copolymer comprising (a1) (0.5-15, preferably 1-7 mole.%). (c1) has a weight average molecular weight of 1000-10000000.

Preferred Substrate: In (M2), the substrate surface is the surface of a primer layer that is supported by a support layer and the substrate is a substrate for a biochip. (S1) is the surface of

a primer layer that is supported on the supporting layer, is planar and is a biochip. (S1) comprises a supporting layer that comprises a material selected from polymer or composite; polymer and is electrically conductive. In (S1), the primer layer is a hydrophobic primer layer (preferably a silane primer layer, a hydrocarbon silane primer layer, a fluorinated silane primer layer, a mixed fluorinated/hydrocarbon silane primer layer, or a polymeric primer layer). The primer layer is 4 Angstrom-3 microm (preferably 4 Angstrom- 10 nm) thick. In (S1), the hydrogel is present on the surface only in at least one discreet spots (preferably several discreet spots having at least one lateral dimension that is 100 nm-3 mm). The lateral dimension is 500 nm-500 microm.

Preferred Method: In (M2), the photocross-linking is selective, such that some of the hydrogel precursor is photocross-linked and some of the hydrogel precursor is not exposed. The selective photocross-linking provides discreet spots of photocross-linked hydrogel. In (M2), the surface comprises photoreactive functionality and the photocross-linking comprises exposing predetermined areas of the surface to photocross-linking conditions, so that the photocross-linkable functionality cross-links to generate a cross-linked polymeric hydrogel, thus the photoreactive functionality covalently binds the cross-linked polymeric hydrogel in the areas.

ORGANIC CHEMISTRY - Preferred Components: The photocross-linkable functionality is a ultraviolet (UV)-curable functionality; at least one of benzophenone, diazoester, arylazide, and diazirine, or their derivatives (preferably benzophenone groups or their derivatives); comprises a carbonyl group. The chemically selective functionality is covalently or electrostatically reactive with protein under aqueous conditions. The chemically selective functionality is an electrophilic or nucleophilic group; an anionic or a cationic group (preferably carboxylic acid, quaternary ammonium salt, alkylarylethyleneoxy, or ketone, or carboxylic acid, amino, or quaternary amino group). The metal ion complexing moiety is selected from N,N-bis (carboxymethyl)-L-lysine, iminodiacetic acid, aminohydroxamic acid, salicylaldehyde, 8-hydroxy-quinoline, N,N,N'-tris(carboxytrimethyl)ethanolamine and N-(2-pyridylmethyl) aminoacetate. The third monomer subunit comprises an energy absorbing moiety (selected from benzoic acid, cinnamic acid, succinic acid, sinapinic acid, nicotinic acid and their derivatives); energy absorbing moiety comprising photon absorbing moiety comprising an aryl nucleus that absorbs photo-irradiation from a high fluence source to generate thermal energy, and transfers the thermal energy to allow desorption and ionization of an analyte in operative contact with the hydrogel and energy absorbing moiety that absorbs light from an ultraviolet or infrared laser. The third monomer subunit comprises both an energy absorbing moiety and a chemically selective functionality for binding a protein.

Preferred Method: In (M3), the detection of the biomolecular analyte, which is effected in a mass spectrophotometer probe

(preferably is a gas phase ion spectrometer probe).

Preferred Precursor: (c3) further comprises second monomeric subunits that comprise a chemically selective functionality for binding a biomolecular analyte, which comprises a covalently or non-covalently binding moiety. In (c3), the second monomer subunits comprises a binding moiety selected from biospecific moiety, positively charged moiety, negatively charged moiety, anion exchange moiety, cation exchange moiety, metal ion complexing moiety, metal complex, polar moiety, hydrophobic moiety and reactive organic functional group (preferably amino acid, dye, carbohydrate, nucleic acid, polypeptide, lipid and sugar, especially diethylaminoethyl and triethylamine, sulfonate and carboxylate, particularly epoxy, imidizole, N-hydroxy-succinimide, iodoacetyl, thiol and aldehyde); a complexed metal ion.

INORGANIC CHEMISTRY - Preferred Substrate: (S1) comprises a supporting layer that comprises a material selected from the aluminum, silicon, glass, metal oxide, metal and composite, and wherein said surface is a surface of a primer layer that is supported on the supporting layer.

Preferred Components: The metal ion is copper, iron nickel cobalt, gallium or zinc.

Preferred Particle: The particle comprises a non-hydrogel particle coated with the hydrogel; is free of non-hydrogel material.

BIOTECHNOLOGY - Preferred Components: In (c3), the binding moiety is selected from antibody, antigen, ligands for receptors, receptors, heparin, biotin, avidin, and streptavidin.

EXTENSION ABSTRACT:

EXAMPLE - A photocross-linkable copolymer having (photocross-linkable group (10 mol.%) was prepared as follows: 3-(methacryloylamino) propyl-trimethylammonium chloride solution (22 g) were mixed with distilled water (30 g) followed with 2-(acryloyloxy) ethyl) (4-benzoylbenzyl) dimethylammonium bromide (2.32 g), V-50 (RTM) (0.045 g), a water-soluble, cationic azo-initiator. The solution was purged with a flow of argon for five minutes. The vessel was sealed and then heated at 58 degreesC for 40 hours. The solution became very viscous after polymerization. The solution was concentrated under vacuum, and then the reaction mixture was dialyzed against deionized water through a seamless cellulose tube. The dialyzed polymer solution was freeze-dried under vacuum to obtain a white solid of the product. The solid powder of polymer was stored in brown vessel and used without further purification. Aluminum substrate was chemically cleaned with 0.01 N HCl and methanol in an ultrasonic bath for 40 minutes, respectively. After wet cleaning, aluminum substrate was further cleaned with ultraviolet (UV)/ozone cleaner for 30 minutes. In the following CVD silanation process, the aluminum substrate was placed in a reaction chamber along with 3-(trimethoxysilyl)propyl methacrylate. A vacuum was pulled on the chamber, and the silane vaporized and reacted with the surface. The reaction was kept for 48 hours for completion. The formation of methacrylate-coated silane layers on the surface was confirmed with surface reflectance and contact angle measurements. An aqueous solution (10 %, by weight) of the obtained copolymer having 10 mol.% of photocross-linkable groups along the polymer backbone were dispensed on the surface of methacrylate-coated aluminum substrates, respectively. The substrate was then subjected to a process of spin-coating at 3,000 revolution per minutes (rpm) for

one minute. The polymer-coated chips then was exposed for 20 minutes to UV light of 360 nm in wavelength. Reflectance FTIR spectra confirmed the formation of SAX (RTM; biochip) hydrogel coating on the surface of aluminum substrate. To check the stability of SAX (RTM) hydrogel coatings on the surface of aluminum substrate, SAX (RTM) polymeric hydrogel-coated chips were immersed in deionized water for 24 hours, and surface reflectance FTIR was used to follow this experiment. FTIR spectra showed, that there was no decrease in IR peak intensity of hydrogel coatings after 24 hours water immersion. The results indicated that the hydrogels remained on the surface after 24 hours water immersion, and even an as low as 3 mol .% of photocross-linkable group incorporated into the polymer backbone was able to fix the polymeric coating on the surface of the substrates completely. In a control experiment, the SAX (RTM) polymeric coating was prepared on non-pretreated aluminum substrates (i.e. the aluminum substrate was not subjected to the treatment of CVD silanation) and subjected to UV curing. The polymeric coating, however, did not stay on the surface of the substrate after washing with water.

FILE SEGMENT: CPI; GMPI

MANUAL CODE: CPI: A04-D04A1; A04-F06E5; A04-F06E7; A12-V00V; B04-B01B; B04-B04C; B04-B04D4; B04-B04D5; B04-C02; B04-C03; B04-E01; B04-G01; B04-N04; B04-N06; B05-A01B; B05-A03A; B05-B02C; B06-D02; B06-F03; B07-D04C; B10-A13D; B10-A22; B10-B01B; B10-B02J; B10-C02; B10-C04C; B10-E02; B11-C04; B11-C08A; B12-K04A; D05-H09; D09-C01; G02-A05

L25 ANSWER 6 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN

ACCESSION NUMBER: 2004-642213 [62] WPIX

DOC. NO. CPI: C2006-036473 [11]

DOC. NO. NON-CPI: N2006-087743 [11]

TITLE: Identifying drug non-target biomolecules in mixture

of biomolecules involves interacting mixture of biomolecules with capture compounds having high binding affinity and analyzing captured biomolecules to identify drug non-targets

DERWENT CLASS: A89; B04; C07; D16; S03; T01

INVENTOR: GREALISH M P; HASSMAN C F; HASSMAN III C F; KOESTER H; KOSTER H; LITTLE D P; MARAPPAN S; SIDDIQI S M; YIP P

PATENT ASSIGNEE: (GREA-I) GREALISH M P; (HASS-I) HASSMAN C F; (HKPH-N) HK PHARM INC; (KOES-I) KOESTER H; (KOST-I) KOSTER H; (LITT-I) LITTLE D P; (MARA-I) MARAPPAN S; (SIDD-I) SIDDIQI S M; (YIPP-I) YIP P

COUNTRY COUNT: 107

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2004064972	A2	20040805	(200462)*	EN	368[38]	
US 20050042771	A1	20050224	(200515)	EN		
AU 2004206856	A1	20040805	(200557)	EN		
EP 1583972	A2	20051012	(200567)	EN		
US 20060051879	A9	20060309	(200618)	EN		

IN 2005MN00902	P3	20051007 (200639)	EN	
JP 2006518450	W	20060810 (200654)	JA	248
AU 2004206856	B2	20060907 (200712)	EN	
AU 2004206856	B9	20061102 (200725)	EN	
AU 2006249219	A1	20070111 (200733)#	EN	
AU 2004206856	A8	20070607 (200765)	EN	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2004064972 A2		WO 2004-US1037	20040116
US 20050042771 A1	Provisional	US 2003-441398P	20030116
US 20060051879 A9	Provisional	US 2003-441398P	20030116
AU 2004206856 A1		AU 2004-206856	20040116
AU 2004206856 B2		AU 2004-206856	20040116
AU 2004206856 B9		AU 2004-206856	20040116
AU 2006249219 A1	Div Ex	AU 2004-206856	20040116
EP 1583972 A2		EP 2004-702919	20040116
US 20050042771 A1		US 2004-760085	20040116
US 20060051879 A9		US 2004-760085	20040116
EP 1583972 A2		WO 2004-US1037	20040116
IN 2005MN00902 P3		WO 2004-US1037	20040116
JP 2006518450 W		WO 2004-US1037	20040116
IN 2005MN00902 P3		IN 2005-MN902	20050816
JP 2006518450 W		JP 2006-500969	20040116
AU 2006249219 A1		AU 2006-249219	20061206
AU 2004206856 A8		AU 2004-206856	20040116

FILING DETAILS:

PATENT NO	KIND		PATENT NO	
AU 2004206856	A1	Based on	WO 2004064972	A
EP 1583972	A2	Based on	WO 2004064972	A
JP 2006518450	W	Based on	WO 2004064972	A
AU 2004206856	B2	Based on	WO 2004064972	A
AU 2004206856	B9	Based on	WO 2004064972	A
AU 2004206856	A8	Based on	WO 2004064972	A

PRIORITY APPLN. INFO: US 2003-441398P 20030116
US 2004-760085 20040116
AU 2006-249219 20061206

INT. PATENT CLASSIF.:

MAIN: B01D

IPC ORIGINAL: C07C0069-00 [I,C]; C07C0069-00 [I,C]; C07C0069-76 [I,A]; C07C0069-96 [I,C]; C07C0069-96 [I,A]; C07D0207-00 [I,C]; C07D0207-00 [I,C]; C07D0207-404 [I,A]; C07D0207-46 [I,C]; C07D0207-46 [I,A]; C07D0209-00 [I,C]; C07D0209-00 [I,C]; C07D0209-48 [I,A]; C07D0211-00 [I,C]; C07D0211-00 [I,C]; C07D0211-60 [I,A]; C07D0211-78 [I,C]; C07D0211-78 [I,A]; C07D0213-00 [I,C]; C07D0213-00 [I,C]; C07D0213-79 [I,A]; C07D0215-00 [I,C]; C07D0215-00 [I,C]; C07D0215-48 [I,A]; C07D0239-00 [I,C]; C07D0239-00 [I,C]; C07D0239-54 [I,A]; C07D0239-545 [I,C]; C07D0239-545 [I,A]; C07D0241-00 [I,C]; C07D0241-00 [I,C]; C07D0241-44 [I,A]; C07D0261-00 [I,C]; C07D0261-00 [I,C]; C07D0261-12 [I,A]; C07D0271-00 [I,C]; C07D0271-00 [I,C]; C07D0271-07

[I,A]; C07D0303-00 [I,C]; C07D0303-00 [I,C];
C07D0303-14 [I,A]; C07D0303-16 [I,C]; C07D0303-16
[I,A]; C07D0317-00 [I,C]; C07D0317-00 [I,C];
C07D0317-36 [I,A]; C07D0401-00 [I,C]; C07D0401-00
[I,C]; C07D0401-12 [I,A]; C07D0405-00 [I,C];
C07D0405-00 [I,C]; C07D0405-10 [I,A]; C07D0405-12
[I,C]; C07D0405-12 [I,A]; C07D0495-00 [I,C];
C07D0495-00 [I,C]; C07D0495-04 [I,A]; C07D0498-00
[I,C]; C07D0498-00 [I,C]; C07D0498-18 [I,A];
C07D0519-00 [I,C]; C07D0519-00 [I,A]; C07D0519-00
[I,C]; C12N0015-09 [N,A]; C12N0015-09 [N,C];
G01N0027-62 [I,A]; G01N0027-62 [I,C]; G01N0030-00
[I,C]; G01N0030-72 [I,A]; G01N0033-15 [I,A];
G01N0033-15 [I,C]; G01N0033-50 [I,A]; G01N0033-50
[I,C]; G01N0033-53 [I,A]; G01N0033-53 [I,C];
G01N0033-543 [I,A]; G01N0033-543 [I,C]; G01N0033-
68
[I,C]; G01N0033-68 [I,A]; G01N0033-68 [I,C];
G01N0037-00 [I,A]; G01N0037-00 [I,C]

IPC RECLASSIF.: C07C0069-00 [I,C]; C07C0069-76 [I,A]; C07C0069-96 [I,A]; C07D0207-00 [I,C]; C07D0207-404 [I,A]; C07D0207-46 [I,A]; C07D0209-00 [I,C]; C07D0209-48 [I,A]; C07D0211-00 [I,C]; C07D0211-60 [I,A]; C07D0211-78 [I,A]; C07D0213-00 [I,C]; C07D0213-79 [I,A]; C07D0215-00 [I,C]; C07D0215-48 [I,A]; C07D0239-00 [I,C]; C07D0239-54 [I,A]; C07D0239-545 [I,A]; C07D0241-00 [I,C]; C07D0241-44 [I,A]; C07D0261-00 [I,C]; C07D0261-12 [I,A]; C07D0271-00 [I,C]; C07D0271-07 [I,A]; C07D0303-00 [I,C]; C07D0303-14 [I,A]; C07D0303-16 [I,A]; C07D0317-00 [I,C]; C07D0317-36 [I,A]; C07D0401-00 [I,C]; C07D0401-12 [I,A]; C07D0405-00 [I,C]; C07D0405-10 [I,A]; C07D0405-12 [I,A]; C07D0495-00 [I,C]; C07D0495-04 [I,A]; C07D0498-00 [I,C]; C07D0498-18 [I,A]; C07D0519-00 [I,A]; C07D0519-00 [I,C]; G01N0033-68 [I,A]; G01N0033-68 [I,C]

BASIC ABSTRACT:

WO 2004064972 A2 UPAB: 20060122

NOVELTY - Identifying drug non-target biomolecules in mixture of biomolecules, comprising interacting mixture with capture compounds having moiety X which covalently binds to biomolecules or with high affinity, moiety Y that increases selectivity of binding so that the capture compound binds to fewer biomolecules, and moiety Z for presenting X and Y, and analyzing captured biomolecules to identify drug non-targets.

DETAILED DESCRIPTION - Identifying (M1) drug non-target biomolecules in mixture of biomolecules, by: (a) interacting mixture of biomolecules with a capture compound or a collection of compounds, where each set of capture compounds includes a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of bimolecular/capture compounds are stable under conditions of mass spectrometric analysis, a moiety Y that increases the selectivity of the binding by X so that the capture compound binds to fewer biomolecules when the selectivity moiety is present than in its absence, and a moiety Z for presenting X and Y and/or a moiety Q, where Q permits sorting; and

(b) analyzing the captured biomolecules to identify drug non-targets.

INDEPENDENT CLAIMS are also included for the following: (1) a

collection of capture compounds (CC); (2) a system (S) for analysis of mixtures of biomolecules, comprising:
(a) CC;
(b) a computer programmed with instructions for controlling and directing analysis of biomolecules using the collections; (c) mass spectrometer; and
(d) software for analysis of data produced by the mass spectrometer;
(3) processing (M2) the mass spectrometric data produced using CC;
(4) a solid support comprising CC, where each set of compounds is arrayed at a single locus; and (5) re-designing (M3) a drug, comprising: (a) contacting CC comprising a drug with a sample containing biomolecules to effect capture of biomolecules in the sample; and (b) isolating and identifying the captured biomolecules, and to eliminate or alter its binding interactions with a captured biomolecule.
R15 = a monovalent group chosen from straight or branched alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, cycloalkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, aryl, arylalkyl, arylalkenyl, arylalkynyl, heteroaryl, heteroarylalkyl, heteroarylalkenyl, heteroarylalkynyl, halo, haloalkyl, pseudohalo, azido, cyano, nitro, OR60, NR60R61, COOR60, C(O)R60, C(O)NR60R61, S(O)qR60, S(O)qOR60, S(O)qNR60R61, NR60C(O)R61, NR60C(O)NR60R61, NR60S(O)qR60, SiR60R61R62, P(R60)2, P(O)(R60)2, P(OR60)2, P(O)(OR60)2, P(O)(OR60)(R61) or P(O)NR60R61; and
l, m and n = 0-4.
Where all l, m and are not equal to 0 at the same time.

USE - CC is useful for analysis of biomolecule comprising contacting a composition of a biomolecule with CC to form capture compound-biomolecule complexes, and/or digesting the captured biomolecules by chemical or enzymatic treatment, separating each set of captured compounds based on the sorting moiety Q, analyzing each set of capture compounds to identify the biomolecules, and identifying or detecting bound biomolecules. This comprises mass spectrometric analysis of bound biomolecules. Biomolecules bound to the capture compounds are treated with a protease prior to mass spec analysis. Each set of compounds comprises the same reactivity function but differs in selectivity function. CC is useful for separating protein conformers, by contacting a composition comprising a biomolecule with CC, separating members of the collection, and identifying the bound proteins from the mixture, where each conformer has different binding specificity for members of the collection. At least one conformer is associated with a disease. CC is useful for reducing diversity of complex mixture of biomolecules, comprising contacting the mixture with CC to form complexes of capture compounds with bound biomolecules, and either before, during or after contacting, separating each set of complexes of capture compounds with biomolecules from the other sets. CC is useful for identification of phenotype-specific biomolecules, comprising sorting cells from a single subject according to a predetermined phenotype to produce at least two separated sets of cells, contacting mixtures of biomolecules from each set of sorted cells with CC, and comparing the patterns of biomolecules binding from each set to identify biomolecules that differ for each set. The cells are synchronized or frozen in a metabolic state before sorting and/or after sorting. The phenotypes are diseased or healthy. A disease phenotype is a tumor and a healthy phenotype is non-tumor. The contacting step is performed in an aqueous or hydrophobic medium and the biomolecules are hydrophilic or hydrophobic. The identification or detection is by mass spectrometric analysis of the biomolecule-capture compound complexes. The mass

spectrometric format is matrix assisted laser desorption ionization-time of flight (MALDI- TOF) mass spectrometry. It further involves chemical or enzymatic treatment of the biomolecule-capture compound complexes to remove or cleave its portions. The mass spectrometric analysis of the bound biomolecules, comprises addition of matrix to the sets of biomolecule-capture agent complexes, and MALDI-TOF mass spectrometry of each set of biomolecule-capture agent complexes. The composition is a cell lysate. CC is useful for analyzing biomolecule interactions which involves contacting a mixture of biomolecules with CC to form a compound-biomolecule complexes, where the central core is not cleavable prior to or during mass spectrometric analysis of biomolecules bound to the capture compound, and the complexes are stable to MALDI-TOF mass spectrometry conditions, contacting the capture compound-biomolecule complexes with a mixture containing compounds chosen from mixtures of biomolecules and small molecules test compounds, where compounds in the mixture bind to biomolecules in the complexes, before or after the contacting steps immobilizing the capture compounds on a solid support through the sorting group of each set of capture compounds, and analyzing the bound compounds by mass spectrometry. The small molecule test compounds are candidates drugs and are chosen from small organic molecules, peptides, peptide mimetics, antisense molecules or dsRNA, antibodies, fragments of antibodies and recombinant or synthetic antibodies and their fragments, and the method comprises identifying candidate drugs that bind to biomolecules. The capture compound-biomolecule of biomolecules and small molecules test compounds, are contacted with a mixture of biomolecules to identify components of biomolecule complexes or pathways (all claimed). DESCRIPTION OF DRAWINGS - The drawing shows schematic depiction of the apparatus for analyzing mixture of biomolecules. TECHNOLOGY FOCUS:

BIOTECHNOLOGY - Preferred Method: In (M1), the moiety Y is a pharmaceutical drug, drug fragment, drug metabolite or prodrug, the moiety Y is linked to the moiety Z in different orientations through different points of attachments on the moiety. The biomolecules are proteins, receptors or enzymes. Q permits separation of capture compounds by arraying of the capture compounds on a solid support by binding to the surface or its molecule. The set of capture compounds includes at least 10, 50, preferably 100 different capture compounds. Q is chemical group for arraying at addressable loci on solid supports. The component capture compounds are chosen from compound that has the formula called (2) or from the formulae Q-Z1-(X)m and Q-Z1-(Y)n.

Z1 = moiety that is cleavable prior to or during mass spectrometric analysis biomolecules bound to the capture compound; and

m and n = 1-100.

The component capture compounds are chosen from compounds that have the formulae: QZX and Q-Z-Y.

Z = oligonucleotide or oligonucleotide analog that includes a single-stranded portion of sufficient length j to form a stable hybrid with a base-complementary single-stranded nucleic acid molecule or analog;

Q = formula N1sBiN2u;

N1, B and N2 = oligonucleotides or oligonucleotide analogs comprising s, t and u members, respectively;

B = a region of sequence permutations that contains at least two bases; and

sum of s, i and u = at least 5.

Each member of N1, B and N2 is chosen from monomer building blocks of deoxyribonucleic acid, ribonucleic acid, protein nucleic acid and their analogs. Z is a photocleavable, acid cleavable, alkaline cleavable, oxidatively cleavable, or reductively cleavable group. Z comprises an insoluble support to which each X, Y and Q is linked either directly or through a linker. The insoluble support is chosen from bead, capillary, plate, membrane, wafer, comb, pin, a wafer with pits, an array of pits or nanoliter wells and a flat surface for receiving or linking samples at discrete loci. The support comprises silicon, silica gel, glass, nylon, Wang resin, Merrifield resin, dextran cross-linked with epichlorohydrin, agarose, cellulose, magnetic beads, Dynabeads, a metal surface or a plastic material. Z comprises hydrophobic beads comprising polystyrene, polyethylene, polypropylene or teflon, or hydrophilic beads comprising cellulose, dextran cross-linked with epichlorohydrin, agarose, polyacrylamide, silica gel and controlled pore glass. The Z moiety comprises spacer groups S1 and/or S2, and a cleavable linkage, where the S1 and/or S2 moieties are attached to insoluble support and the cleavable linkage is attached to S2, if present, otherwise to the insoluble support.

Z = at least a trivalent moiety chosen from alkylene, alkenylene, alkynylene, alkylenoxy, alkylenthio, alkylencarbonyl, alkylenamino, cycloalkylene, cycloalkenylene, cycloalkynylene, cycloalkylenoxy, cycloalkylenthio, cycloalkylencarbonyl, cycloalkylenamino, heterocyclylene, arylene, arylenoxy, arylenthio, arylencarbonyl, arylenamino, heteroarylene, heteroarylenoxy, heteroarylenthio, heteroarylencarbonyl, heteroarylenamino, oxy, thio, carbonyl, carbonyloxy, ester, amino, amido, phosphino, phosphineoxido, phosphoramidato, phosphinamidato, sulfonamido, sulfonyl, sulfoxido, carbamato, ureido, and their combinations, and is unsubstituted or substituted with one or more substituents each chosen from R15 as described above;

q = 0-2;

each R60, R61 and R62 = hydrogen, alkyl, alkenyl, alkynyl, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl or heteorcyclylalkynyl.

Where Z is cleavable prior to or during analysis of the biomolecule.

Z = at least a trivalent moiety and is chosen from straight or branched chain alkyl, alkenyl, alkynyl, (C(R15)2)d, O, S, (CH2)d, (CH2)dO, (CH2)dS, greater than N(R15), (S(O)u), (S(O)2)w, greater than C(O), (C(O))w, (C(S(O)u))w, (C(O)O)w, (C(R15)2)dO, (C(R15)2)dS(O)u, O(C(R15)2)d, S(O)u(C(R15)2)d, (C(R15)2)dO(C(R15)2)d,(C(R15)2)dS(O)u(C(R15)2)d, N(R15)(C(R15)2)d, (C(R15)2)dNR15, (C(R15)2)dN(R15)(C(R15)2)d, -(CH2)dC(O)N(CH2)d-, -(CH2)dC(O)N(CH2)dC(O)N(CH2)d-, (S(R15)(Ou)w, (C(R15)2)d, (C(R15)2)dO(C(R15)2)d,(C(R15)2)d(C(O)O)w(C(R15)2)d, (C(O)O)w(C(R15)2)d, (C(R15)2)d(C(O)O)w, (C(S)(R15)w, (C(O))w(CR152)d, (CR15)d(C(O))w(CR15)d, (C(R15)2)d(C(O))w, N(R15)(C(R15)2)w, OC(R15)2C(O), O((R15)2C(O)N(R15),

(C(R15)2)wN(R15)(C(R15)2)w, (C(R15)2)wN(R15), greater than P(O)v(R15)x, greater than P(O)u(R15)3, greater than P(O)u(C(R15)2)d, greater than Si(R15)2 and their combinations;

u, v and x = 0-5;

each d = 1-20, preferably 1-3; and

each w = 1-6, preferably 1-2.

Where Z is cleavable prior to or during analysis of the biomolecule.

Z = trivalent moiety having any combination chosen from arylene, heteroarylene, cycloalkylene, greater than C(R15)2, C(R15)=C(R15), greater than Cequivalent toC(R23)(R24), greater than C(R23)(R24), Cequivalent toC, O, greater than S(A)u, greater than P(D)v(R15), greater than P(D)v(ER15), greater than Si(R15)2, greater than N(R15), greater than N+(R23)(R24) and greater than C(E);

u = 0, 1 or 2;

v = 0, 1, 2 or 3;

A = O or NR15;

D = S or O; and

E = S, O or NR15.

Where the groups can be combined in any order:

each R15 = monovalent group chosen from hydrogen and Y1R18;

each Y1 = a divalent group having any combination of the following groups: a direct link, arylene, heteroarylene, cycloalkylene, greater than C(R17)2, C(R17)=C(R17), greater than C=C(R23)(R24), greater than C(R23)(R24), Cequivalent toC, O, greater than S(A)u, greater than P(D)v(R17), greater than P(D)v(ER17), greater than N(R17), greater than N(COR17), greater than N+(R23)(R24), greater than Si(R17)2 and greater than C(E);

R17 and R18 = hydrogen, halo, pseudohalo, cyano, azido, nitro, SiR27R28R25, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and NR19R20;

R19 and R20 = hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl and heterocyclyl; R23 and R24 = R23 and R24 are chosen from hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl and heteroaryl; or R23 and R24 together form alkylene, alkenylene or cycloalkylene;

R25, R27 and R28 = monovalent group chosen from hydrogen, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and NR19R20;

R15, R17,-R20, R23-R25, R27 and R28 = substituted with one or more substituents each chosen from Z2;

Z2 = alkyl, alkenyl, alkynyl, aryl, cycloalkyl, cycloalkenyl, hydroxy, S(O)hR35;

h = 0, 1 or 2, NR35R36, COOR35, COR35, CONR35R36, OC(O)NR35R36, N(R35)C(O)R36, alkoxy, aryloxy, heteroaryl, heterocyclyl, heteroaryloxy, heterocyclyloxy, aralkyl, aralkenyl, aralkynyl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl,

aralkoxy, heteroaralkoxy, alkoxycarbonyl, carbamoyl, thiocarbamoyl, alkoxycarbonyl, carboxyaryl, halo, pseudohalo, haloalkyl and carboxamido; and

R35 and R36 = hydrogen, halo, pseudohalo, cyano, azido, nitro, trialkylsilyl, dialkylarylsilyl, alkyldiarylsilyl, triarylsilyl, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy, amino, amido, alkylamino, dialkylamino, alkylarylamino, diarylamino and arylamino.

Z has the formula: (S1)tM(R15)a(S2)bL.

S1 and S2 = spacer moieties;

t and b = each independently 0 or 1;

a = 0-4;

M = central moiety possessing three or more points of attachment;

R15 = monovalent group chosen from Y2R18; and

L = group that is cleavable prior to or during mass spectrometric analysis of the compound. M is a tetravalent alkylene, tetravalent phenylene, tetravalent biphenylene or a tetravalent heterobifunctional trityl derivative, and is unsubstituted or is substituted with 1-4 groups, each chosen from R15;

M = at least a trivalent group chosen from any one of the groups having the formulae called (3-20) lacking a hydrogen atom: (CH2)r, (CH2O)r, (CH2CH2O)r, (NH(CH2)rC(=O))s, (NHCH(R52)C(=O))r and (O(CH)rC(=O))s.

r and s = 1-10;

R52 = side chain of a natural or unnatural alpha-amino acid;

z = 1-4;

l, m and n = 0-4;

S1 and S2 = any one of formulae called (21-25): (CH2)r, (CH2O), (CH2CH2O)r,(NH(CH2)rC(=O))s and (NHCH(R52)C(=O))s)(O(CH)rC(=O))s.

L = disulfide moiety, a photocleavable group, an acid cleavable group, an alkaline cleavable group, a oxidatively cleavable group, or a reductively cleavable group, a trityl ether, an ortho nitro substituted aryl group, an o-nitrobenzyl, a phenacyl, nitrophenylsulfenyl group, or formula I, II or III.

R20 = (omega)(4,4'dimethoxytrityloxy)alkyl or (omega)hydroxyalkyl;

R21 = hydrogen, alkyl, aryl, alkoxycarbonyl, aryloxycarbonyl and carboxy;

R22 = hydrogen;

t = 0-3;

R50 = alkyl, alkoxy, aryl or aryloxy;

X20 = hydrogen, alkyl or OR20;

R1 = hydrogen;

R2 = (omega)hydroxyalkoxy, (omega)(4,4'-dimethoxytrityloxy)alkoxy, (omega)hydroxyalkyl and (omega)(4,4'-dimethoxytrityloxy)alkyl, or (un)substituted on alkyl or alkoxy chain with one or more alkyl groups; and

c and e = 0-4;

L = SS, OP(=O)(OR51)NH, pMeoNO2PhCH2, OC(=O), and formulae called 26-30.

R51 = straight or branched chain alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, aralkyl, aralkenyl,

aralkynyl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, cycloalkylalkyl, cycloalkylalkenyl, cycloalkylalkynyl, heterocyclylalkyl, heterocyclylalkenyl or heterocyclylalkynyl; and y = 0-4;

R15 = H, OH, OR51, SH, SR51, NH2, NHR51, N(R51)2, F, Cl, Br, I, SO3H, PO24, CH3, CH2CH3 or CH(CH3)a or C(CH3)3;

X = active ester, an active halo moiety, an amino acid side chain-specific functional group, a reagent that binds to active site of an enzyme, a ligand that binds to a receptor, a specific peptide that binds to a biomolecule surfaces, a lectin, an antibody, an antigen, biotin and streptavidin. X is alpha-halo ether, an alpha-halo carbonyl group, maleimido, a metal complex, an epoxide, an isothiocyanate, or an antibody against phosphorylated or glycosylated peptides/proteins; or C(=O)OphpNO2, C(=O)OC6F5, C(=O)O(N succinimidyl), OCH2I, OCH2Br, OCH2Cl, C(O)CH2I, C(O)CH2Br or C(O)CH2Cl; or any one of formulae called 31-37.

The member compounds comprise a mass modifying tag linked to Z or is S2. The mass modified Z moiety has the formula: (S1)tM(R15)a(S2)bLT, where T is a mass modifying tag. The mass modifying tag is a divalent group having the formula X1R10 and is chosen from:

(a) X1 is a divalent group chosen from O, OC(O)(CH2)yC(O)O, NHC(O), C(O)NH, NHC(O)(CH2)yC(O)O, NHC(S)NH, OP(O-alkyl)O, OSO2O, OC(O)CH2S, S, NH and a formula called (38), R10 is a divalent group chosen from (CH2CH2O)zCH2CH2O, (CH2CH2O)zCH2CH2Oalkylene, alkylene, alkenylene, alkynylene, arylene, heteroarylene, (CH2)zCH2O, (CH2)2CH2Oalkylene, (CH2CH2NH)zCH2CH2NH, CH2CH(OH)CH2O, Si(R12)(R13), CHF and CF2; where y is 1-20; z is 0-200; R11 is the side chain of a naturally occurring alpha-amino acid; and R12 is chosen from alkyl, aryl and aralkyl;

(b) SS;

(c) S;

(d) (NH(CH2)yNHC(O)(CH2)yC(O))zNH(CH2)y NHC(O)-(CH2)yC(O)O, where y and z are selected as in (i);

(e) (NH(CH2)yC(O))zNH(CH2)yC(O)O;

(f) (NHCH(R11)C(O))zNHCH(R11)C(O)O; or

(g) (O(CH2)yC(O))zNH(CH2)yC(O)O. S2 has the formula X1R10.

CC comprises a central core Z linked to a reactive functionality X and a selectivity functionality Y, where CC a covalent bond with a biomolecule in the mixture or interacts with high stability such that the affinity of binding of the capture compound to the biomolecule through the reactive functionality in the presence of the selectivity functionality is at least ten-fold greater than in the absence of the selectivity functionality. The compounds in the collection comprises Z, which comprises a reagent of a luminescence assay or a group that is detected in a colorimetric assay, and a sorting group Q that comprises a single-stranded oligonucleotide. Z is a solid support or particulate support. CC further comprises a solubility group W that influences the solubility properties of the capture compound. The selectivity function Y is a pharmaceutical drug chosen from atorvastatin, celecoxib, refecoxib and cerivastatin. M is any one of formulae called (39-47).

Q is biotin, hexa-His, 4,4-difluoro-4-bora-3a, 4a-diaza-s-indacene, oligonucleotides, nucleosides, nucleotides, antibodies, immunotoxin conjugates, adhesive peptides, lectins, liposomes, protein nucleic acids, activated dextrans or peptides,

preferably biotin. Z has the formula called (48).

CC comprises several capture compounds, comprising sets of capture compounds, where each set of capture compounds includes a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis, a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomolecules when the selectivity moiety is present than in its absence, and a moiety Z for presenting X and Y, where the moiety Z is represented by a formula called (1).

M2 comprises subtracting any background reducing noise, calibrating molecular weight, and refining peaks; In (M2), the step of refining peaks comprises peak integration. (M2) further involves comparing the processed data with existing protein databases or DNA databases containing open reading frames to determine whether the protein is known, and if the protein is known, identifying modifications, comparing data from tissues of healthy and diseased individuals, or from different physiological or developmental stages, or from different parts of a tissue to form double stranded hybrids and analyzing the double stranded hybridized complexes. The analysis is orthogonal time of flight (O-TOF) mass spectrometry, or electrospray (ES) mass spectrometry. (M3) further involves identifying a function of a captured biomolecule, where the alteration in binding is an increase or decrease in binding. The biomolecule for which binding is altered is a non-target biomolecule. The biomolecules comprise proteins. The sample comprises a body tissue or fluid. The sample is contacted with CC. The compound comprises an azide, diazirine, or a group, which, following activation, reacts with a hydroxy, amino, thiol or carboxy group of the biomolecule. (M3) is repeated with the re-designed drug linked to a capture compound to effect further modification. The capture compounds bind to the drug at a several sites. The captured proteins are drug target proteins or non-drug target proteins. The concentration of capture compound is varied in several different reactions, and the Kd value is determined. The detection format is linear time-of-flight (TOP), reflectron time-of-flight, single quadruple, multiple quadruple, single magnetic sector, multiple magnetic sector, Fourier transform, ion cyclotron resonance (ICR), or ion trap. The function of a biomolecule is determined by in silico, in vitro, or in vivo methods such as sequence alignment, pharmacophores, homology models and protein motif correlation, liver midrosomes metabolic pathways, cDNA-expressed enzymes, signal pathways and back-mapping to yeast pathways, simulations and protein/protein interaction of pull-out proteins, native polymorphisms, knock-out/knock-in, flow

cytometry,
therapeutic activity of the drug, or prospective genotyping and prospective phenotyping. The redesigning of drug results in a second drug with fewer side-effects or an increased therapeutic index as compared to the first drug. The drug is chosen from troglitazone, rosiglitazone, pioglitazone, methotrexate, atorvastatin, celecoxib, refecoxib and cerivastatin. The compound comprises an active ester group, alkylating agent, active halide or
active pseudohalide. The treatment comprises change in pH. Preferred System: (S) further comprises a liquid chromatographic device.

EXTENSION ABSTRACT:

EXAMPLE - Three different capture compounds (designated HKC 1343, 1349, 1365) were reacted individually with lysozyme. The capture experiments were analyzed using MALDI-TOF mass spectrometry. Binding was performed in 20 microL sample volumes with a 5 microM lysozyme concentrations in 25 mM HEPES buffer solution, pH 7.0. The trityl-based capture compounds were added to the protein solution at a 10 microM concentrations. The binding reaction was incubated at room temperature for 30 minutes. The reaction was quenched using 1 microL of a 100 mM TRIZMA base solution. The capture compound-protein binding mixture was prepared for mass spectrometry by mixing a 1 microL aliquot of a binding reaction with 1 microL of a 10 mg/ml sinapinic acid in 30 % aqueous acetonitrile. The sample was deposited as a 500 nl spot on the surface of the mass target plates and air-dried before mass spectrometric analysis. The results of the mass spectrometry analysis, demonstrate that addition of selectivity groups to compounds permits alterations in the binding specificity of capture compounds.

FILE SEGMENT: CPI; EPI
MANUAL CODE: CPI: A12-L04A; B04-B03C; B04-E01; B04-E05; B04-E10;
B04-F01; B04-G01; B04-K01; B04-L01; B04-N04; B11-B;
B11-C08A; B11-C08B; B11-C08D3; B11-C08E; B11-C08F4;
B12-K04; C11-B; C11-C08A; C11-C08B; C11-C08D3;
C11-C08E; C11-C08F4; C12-K04; D05-H09; D05-H10; D05-H11
EPI: S03-E10A8; S03-E14A1; S03-E14H; T01-J06A; T01-S03

L25 ANSWER 7 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2004-375547 [35] WPIX
DOC. NO. CPI: C2004-141179 [35]
DOC. NO. NON-CPI: N2004-298782 [35]
TITLE: Wavelength tunable composite material for, e.g. optical telecommunication systems, includes crosslinked metallopolymer network having polymer backbone including metal atoms
DERWENT CLASS: A13; A14; A89; E11; P81; V07
INVENTOR: ARSENAULT A; MANNERS I; MIGUEZ H; OZIN G A
PATENT ASSIGNEE: (ARSE-I) ARSENAULT A; (MANN-I) MANNERS I; (MIGU-I) MIGUEZ H; (OZIN-I) OZIN G A
COUNTRY COUNT: 105

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2004034134	A1	20040422	(200435)*	EN	79[16]	
US 20040131799	A1	20040708	(200445)	EN		
AU 2003273661	A1	20040504	(200465)	EN		
EP 1549995	A1	20050706	(200544)	EN		
JP 2006504984	W	20060209	(200612)	JA	36	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2004034134	A1	WO 2003-CA1512	20031009
US 20040131799	A1 Provisional	US 2002-416910P	20021009
AU 2003273661	A1	AU 2003-273661	20031009
EP 1549995	A1	EP 2003-757572	20031009
US 20040131799	A1	US 2003-681374	20031009
EP 1549995	A1	WO 2003-CA1512	20031009
JP 2006504984	W	WO 2003-CA1512	20031009
JP 2006504984	W	JP 2004-542118	20031009

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2003273661	A1 Based on	WO 2004034134 A
EP 1549995	A1 Based on	WO 2004034134 A
JP 2006504984	W Based on	WO 2004034134 A

PRIORITY APPLN. INFO: US 2002-416910P 20021009
US 2003-681374 20031009

INT. PATENT CLASSIF.:

IPC ORIGINAL: C08G0077-00 [I,C]; C08G0077-60 [I,A]; G02B0026-00 [I,A]

IPC RECLASSIF.: G02B0006-122 [I,A]; G02B0006-122 [I,C]; G02F0001-01 [I,A]; G02F0001-01 [I,C]; G02F0001-19 [N,A]; G02F0001-21 [I,A]

BASIC ABSTRACT:

WO 2004034134 A1 UPAB: 20060121

NOVELTY - A wavelength tunable composite material includes an ordered array of constituents having refractive index embedded within a crosslinked metallopolymer network having polymer backbone including metal atoms. The ordered array of the constituents has lattice spacing giving rise to Bragg diffraction when the composite material is illuminated.

DETAILED DESCRIPTION - A wavelength tunable composite material comprises an ordered array of first constituents having a first refractive index embedded within a crosslinked metallopolymer network having a second refractive index. The ordered array of first constituents has a lattice spacing giving rise to Bragg diffraction when the composite material is illuminated. The crosslinked metallopolymer network comprises is made of a polymer backbone including metal atoms chemically integrated to the backbone. It has an electronic configuration dependant on the metal atoms that are switchable between electronic configurations. It is expandable and contractible in response to respective controlled uptake and expulsion of a selected fluid by the crosslinked metallopolymer network so that when the crosslinked metallopolymer network takes up the selected fluid it expands

which shifts a Bragg diffraction wavelength to longer wavelengths and when expels the selected fluid it contracts which shifts the Bragg diffraction wavelength to shorter wavelengths. The amount of fluid uptake and expulsion is controlled by controlling the electronic configuration of the cross-linked metallopolymer network. An INDEPENDENT CLAIM is also included for a method of wavelength tuning a composite material comprising producing an ordered array of first constituents and switching the electronic configuration of the crosslinked metallopolymer network so that the crosslinked polymer network changes dimensions and modulates the lattice spacing of the ordered array of first constituents, which shifts the Bragg diffraction wavelength to a pre-selected wavelength.

USE - For use in filters, mirrors, multiplexors, compensators, limitors and switches in optical telecommunication systems, imaging, display, printing, fingerprinting and sensing systems.

ADVANTAGE - The inventive material can be produced to be rapidly and reproducibly wavelength tunable. It has adjustable photonic crystal lattice dimension and has the ability to cause the light of different wavelengths to be efficiently reflected or transmitted across the UV, visible and near infrared regions of the electromagnetic spectrum.

TECHNOLOGY FOCUS:

IMAGING AND COMMUNICATION - Preferred Component: The cross-linked metallopolymer network has segments in which the metal atoms are connected directly to each other. It has a preselected number density and distribution of crosslinks throughout the composite material, and porosity. The first constituents include microparticles of spheres, ellipsoids, rods, sphere containing polyhedra, cubes, or polyhedra having cross-sectional dimensions of 60 nm-100 mum. They include monodisperse microspheres of insulators, and/or semiconductors. The crosslinks in the network are electronically conducting or electronically insulating.

Preferred Method: The top surface of the array of first constituents is overcoated by cross-linked metallopolymer network precursor mixture to 0 nm-100 mm thick. The first constituents are modified to increase the adhesion between the first constituents and the cross-linked polymer network, or between the substrate and the crosslinked metallopolymer network. They form a face-centered cubic arrangement in the composite material.

INORGANIC CHEMISTRY - Preferred Material: The metal atoms are titanium, vanadium, chromium, manganese, iron, cobalt, nickel, copper, niobium, molybdenum, ruthenium, rhenium, platinum, palladium, and rhodium, and/or zinc. They are connected together directly and/or through linking units that impart pre-selected chemical, physical, electrochemical, optical and electronic properties to the cross-linked metallopolymer network. The monodisperse microspheres can be metals.

ORGANIC CHEMISTRY - Preferred Material: The linking units are optionally substituted carbanions, conjugated carbanions, linear olefins, cyclic olefins, acetylenes, phosphines, amines, carbonyls, carbenes, and/or alkoxides. The cross-links in the metallopolymer network are chemical bonds, physical bonds, nanoparticles, surfaces, hydrogen bonds, coordination bonds, electrostatic interactions, hydrophobic interactions, and/or fluorophobic interactions and phase-separated domains.

POLYMERS - Preferred Material: The cross-linked metallopolymer network is formed from the polymerization of a

metal-containing monomer consisting of bridged metallocenophanes. The bridged metallocenophanes are substituted sila-1-ferrocenophanes (preferably dialkylsila-1-ferrocenophanes, alkylalkoxysila-1-ferrocenophanes, dialkoxysila-1-ferrocenophanes, cycloalkylsila-1-ferrocenophanes, diarylsila-1-ferrocenophanes, alkylarylsila-1-ferrocenophanes, alkylalkenylsila-1-ferrocenophanes, and/or alkylalkynylsila-1-ferrocenophanes; or a metal-containing crosslinker of cyclobutylsila-1-ferrocenophane, sila-1,1'-diferrocenophane, 1,2-bis(methylsila-(1)-ferrocenophane)acetylene, 1,4-bis(methylsila-(1)-ferrocenophane)benzene, bis(methylsila-(1)-ferrocenophane)-1,4-diethynylbenzene, and/or 1,2-bis(methylsila-(1)-ferrocenophane)ethane). The cross-linked metallopolymer network is a polymer of polyferrocenylsilanes. The monodisperse microspheres can be polymers (preferably polystyrene or polymethylmethacrylate).

The substrate is made of elastomeric material.

Preferred Composition: The polymerization includes a mixture of 50-100 weight% monomer, 0-30 weight% crosslinker, and 0-20 weight% initiator.

CERAMICS AND GLASS - Preferred Material: The monodisperse microspheres may be made of silica.

EXTENSION ABSTRACT:

EXAMPLE - The materials investigated were planarized composite colloidal photonic crystals comprising ordered fcc arrangement of sub-micrometer disconnected microspheres in a matrix of weakly crosslinked poly(ferrocenylsilane) (PFS), a swellable redox-active metallopolymer gel Kulbaba, M.J. MacLachlan, C.E.B. Evans, I. Manners, Macromol. Chem, Phys, 202, 1768 (2001). The metallopolymer-colloidal crystal composites over deficiences in organic polymer analogues, as well as introduce additional functionality due to the metal-containing metallopolymer used. The crosslinker in the new PFS comprises two polymerizable silaferrocenyl rings appended to the two ends of an electrically conductive, pi-conjugated diethynylbenzene group. Fabrication of the composite material includes: - (i) evaporative deposition of silica colloids; - (ii) 200 C, 12 hours, vacuum; - (iii) treatment with capping agent 1; - (iv) infiltration of monomers 2 and 3, removal of solvent at 300 mm Hg; - (v) sample covered with PTFE sheet, glass slide and bound with binder clips; - (vi) 190 C, 13 hours, N2; and - (vii) careful removal of clips, PTFE and glass cover. - To produce high quality colloidal photonic crystals, highly monodisperse (standard deviation less than 12-3 % of average sphere diameter) silica microspheres of 280 +/- 5 nm diameter (measured by SEM) produced by the controlled hydrolysis of tetra(ethoxy)silane (W. Stober, A, Fink, E.J. Bohn, J. Colloid Interface Sci. 26, 62 (1968)). The polydispersity was further narrowed by 23 fractionation steps, where the microspheres were allowed to settle slightly, and the bottom and top of the suspension were pipetted and discarded. Planar silica colloidal crystals were produced by the evaporative deposition method (P. Jiang, J.F. Bertone, K.S. Hwang, V.L. Colvin, Chemical Mater. 11, 2132 (1999)) on glass microscope slides, and the film on one side of the glass was wiped off.

FILE SEGMENT: CPI; GMPI; EPI
MANUAL CODE: CPI: A06-D; A12-L03; E31-P03
EPI: V07-F02B; V07-K04

ACCESSION NUMBER: 2004-238679 [22] WPIX
DOC. NO. CPI: C2004-093340 [22]
TITLE: Immobilized nitrogen-containing ligand useful in preparing immobilized catalyst for performing, e.g.
hydrogenation reactions, comprises reaction product
of linker-modified nitrogen-containing ligand, and solid support
DERWENT CLASS: A97; B05; E19; J04
INVENTOR: CHEN W; HEMS W P; XIAO J; HEMS W
PATENT ASSIGNEE: (JOHO-C) JOHNSON MATTHEY PLC; (CHEN-I) CHEN W; (HEMS-I) HEMS W P; (XIAO-I) XIAO J
COUNTRY COUNT: 104

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2004014551	A2	20040219	(200422)*	EN	23[0]	
AU 2003248970	A1	20040225	(200456)	EN		
EP 1545772	A2	20050629	(200543)	EN		
JP 2005535693	W	20051124	(200581)	JA	32	
AU 2003248970	A8	20051103	(200629)	EN		
US 20060135355	A1	20060622	(200642)	EN		
EP 1676635	A2	20060705	(200644)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2004014551	A2	WO 2003-GB3306	20030730
AU 2003248970	A1	AU 2003-248970	20030730
AU 2003248970	A8	AU 2003-248970	20030730
EP 1545772	A2	EP 2003-784236	20030730
EP 1545772	A2	WO 2003-GB3306	20030730
JP 2005535693	W	WO 2003-GB3306	20030730
US 20060135355	A1	WO 2003-GB3306	20030730
JP 2005535693	W	JP 2004-527006	20030730
US 20060135355	A1	US 2005-524550	20050815
EP 1676635	A2 Div Ex	EP 2003-784236	20030730
EP 1676635	A2	EP 2006-4827	20030730

FILING DETAILS:

PATENT NO	KIND		PATENT NO	
AU 2003248970	A1	Based on	WO 2004014551	A
EP 1545772	A2	Based on	WO 2004014551	A
JP 2005535693	W	Based on	WO 2004014551	A
AU 2003248970	A8	Based on	WO 2004014551	A
EP 1676635	A2	Div ex	EP 1545772	A

PRIORITY APPLN. INFO: GB 2002-18675 20020812
INT. PATENT CLASSIF.:
MAIN: B01J031-16; C07C211-29
SECONDARY: B01J031-18; B01J031-24; C07B037-04; C07B037-12; C07B053-00; C07C209-42; C07C211-10; C07C213-02; C07C217-56; C07C247-06; C07C251-02; C07C029-136; C07C029-145; C07C033-18; C07C005-02; C07D203-06;

C07D301-03; C07D301-19; C07D301-32

IPC ORIGINAL: B01J0031-00 [I,A]; B01J0031-00 [I,C]; B01J0031-16 [I,C]; B01J0031-18 [I,A]; C07B0037-00 [I,C]; C07B0037-04 [I,A]; C07B0037-12 [I,A]; C07B0053-00 [I,A]; C07B0053-00 [I,C]; C07C0209-00 [I,C]; C07C0209-42 [I,A]; C07C0211-00 [I,C]; C07C0211-27 [I,A]; C07C0217-00 [I,C]; C07C0217-64 [I,A]; C07C0247-00 [I,C]; C07C0247-06 [I,A]; C07C0247-10 [I,A]; C07C0251-00 [I,C]; C07C0251-02 [I,A]; C07C0029-00 [I,C]; C07C0029-145 [I,A]; C07C0005-00 [I,C]; C07C0005-02 [I,A]; C07D0203-00 [I,C]; C07D0203-06 [I,A]; C07D0301-00 [I,C]; C07D0301-03 [I,A]; C07D0301-14 [I,A]; C07D0301-32 [I,A]

IPC RECLASSIF.: B01J0031-16 [I,A]; B01J0031-16 [I,C]; B01J0031-18 [I,A]; B01J0031-24 [I,A]; C07B0053-00 [I,A]; C07B0053-00 [I,C]; C07B0061-00 [I,A]; C07B0061-00 [I,C]; C07C0209-00 [I,C]; C07C0209-42 [I,A]; C07C0211-00 [I,C]; C07C0211-27 [I,A]; C07C0211-29 [I,A]; C07C0213-00 [I,C]; C07C0213-02 [I,A]; C07C0217-00 [I,C]; C07C0217-56 [I,A]; C07C0217-64 [I,A]; C07C0247-00 [I,C]; C07C0247-10 [I,A]; C07C0251-00 [I,C]; C07C0251-02 [I,A]; C07C0029-00 [I,C]; C07C0029-145 [I,A]; C07C0033-00 [I,C]; C07C0033-18 [I,A]; C07D0301-00 [I,C]; C07D0301-03 [I,A]

BASIC ABSTRACT:

WO 2004014551 A2 UPAB: 20060203

NOVELTY - Immobilized nitrogen-containing ligand comprises a reaction product of a linker-modified nitrogen-containing ligand, and a solid support having a site capable of reacting with a functional group of the nitrogen-containing ligand.

DETAILED DESCRIPTION - Immobilized nitrogen-containing ligand comprises a reaction product of a linker-modified nitrogen-containing ligand of formula (I), and a solid support having a site capable of reacting with a functional group of the nitrogen-containing ligand.

R1-R4 = H, optionally saturated 1-10C alkyl, or aryl; X = NR5R6 or N=R5;

Y = NR7R8 or N=R7;

R5-R8 = H, optionally saturated 1-10C alkyl, aryl, urethane or sulfonyl;

One of the R1-R4 is functionalized with a functional group.

INDEPENDENT CLAIMS are also included for: (a) preparing the immobilized ligand of formula (I) by performing a benzoin condensation on a functionalized benzaldehyde to give a functionalized benzoin; reducing the functionalized benzoin to give a functionalized hydrobenzoin; transforming the functionalized hydrobenzoin into a functionalized 1,2-diarylamine; and reacting the functionalized 1,2-diarylamine with a solid support having a site capable of reacting with functionalized 1,2-diarylamine to form an immobilized ligand; and (b) an immobilized catalyst comprising the above immobilized nitrogen-containing ligand, and a metal compound.

USE - Used in the preparation of immobilized catalyst for performing, e.g. hydrogenation reactions, transfer hydrogenation reactions, dihydroxylation reactions, hydrolysis reactions, carbon-carbon bond formation or Suzuki reactions, hydroamination reactions, epoxidations, aziridinations, cycloadditions, hetero-Diels-Alder reactions, hetero-ene reactions, Claisen rearrangements, carbonyl reductions, sigmatropic rearrangements,

additions of nucleophiles to pi-bonds, or addition of nucleophiles to carbonyl groups and ring-opening reactions (claimed).

ADVANTAGE - The catalyst is readily separated from the reaction products and may be re-used if so desired. TECHNOLOGY FOCUS:

ORGANIC CHEMISTRY - Preferred Component: The ligand is reacted with a linker molecule that provides a functional group capable of reaction with the solid support. The solid support includes silica, titania, zirconia, and/or alumina having reactive sites provided by organic compounds comprising carboxylic acids, anhydrides, phosphates, or sulfonates, or metal-organic compounds comprising organic titanates, aluminates, zirconates or organo-functional silanes. It can be an organo-functional silica material prepared by co-hydrolysis of an organo-functional silane and an alkyl silicate and optionally other metal alkoxides.

POLYMERS - Preferred Component: The linker is a polyethylene glycol. The solid support material to which the nitrogen-containing ligand is covalently bonded is a polymer, metal oxide or organo-functional silica material that has sites capable of reacting with said ligand. The sites include halide (such as chlorine, bromine, fluorine, or iodine), hydroxyl, carbonyl, carboxyl, anhydride, carbene, methacryl, epoxide, vinyl, nitrile, mercapto, isocyanate, amine, imine, amide, or imide. The solid support can be a reactive site-containing polystyrene or polystyrene copolymer.

INORGANIC CHEMISTRY - Preferred Component: The metal compound includes scandium, zirconium, hafnium, niobium, tantalum, chromium, molybdenum, tungsten, manganese, technetium, rhenium, iron, cobalt, nickel, copper, silver, aluminum, germanium, antimony, or tin, preferably palladium, platinum, or ruthenium.

EXTENSION ABSTRACT:

DEFINITIONS - Preferred Definition: - R1, R3 = H; - R2, R4 = functional group-containing aryl group; and - R5-R8 = H; or - NR5R6, NR7R8 = amine (N=C) where R6 and R8 are omitted. - The functional group that may be used to bond to the support comprises halogen (consisting of Cl, Br, F or I), hydroxyl, alkoxy, carbonyl, carboxyl, anhydride, carbene, methacryl, epoxide, vinyl, nitrile, mercapto, amine, imine, amide, or imide. EXAMPLE - To a solution of (1R,2R)-1,2-di(3- benzyloxyphenyl)ethane-1,2-diazide (4.77 g) in ethyl ether was added 3.14 g lithium aluminum tetrahydride at 0 degreesC. The resulting suspension was refluxed for 2 hours, and stirred at room temperature overnight. The reaction mixture was then added with saturated sodium sulfate aqueous solution. The solid formed was filtered off and the filtrate was dried and evaporated under reduced pressure. The residue was triturated with hexane to give 4.08 g, 95% yield of (1R,2R)-1,2-di(3-benzyloxyphenyl)ethane-1,2- diamine.

FILE SEGMENT: CPI

MANUAL CODE: CPI: A12-W11K; B04-C03C; B10-A08; B10-A12C; B10-A14; B10-A17; B10-A20; B10-A25; B10-B04A; B10-B04B; E10-A08A; E10-A08C; E10-A12C2; E10-A14B; E10-A17B; E10-B04A2; E10-B04B; E11-A; E11-F; E35; J04-E04

L25 ANSWER 9 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN

ACCESSION NUMBER: 2003-018853 [01] WPIX

DOC. NO. CPI: C2003-004623 [01]

TITLE: New photosensitize compounds useful in photodynamic therapy for treating and diagnosing various conditions

DERWENT CLASS: B02; B03; P34

INVENTOR: DESJARDINS A M; DOLPHIN D; DOLPHIN D H; STERNBERG E D

PATENT ASSIGNEE: (DESJ-I) DESJARDINS A M; (DOLP-I) DOLPHIN D H; (STER-I) STERNBERG E D; (UYBR-N) UNIV BRITISH COLUMBIA

COUNTRY COUNT: 98

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2002076453	A1	20021003	(200301)*	EN	68[9]	
US 20030013696	A1	20030116	(200308)	EN		
AU 2002306912	A1	20021008	(200432)	EN		
US 6894161	B2	20050517	(200533)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2002076453	A1	WO 2002-US9488	20020327
US 20030013696	A1 Provisional	US 2001-279233P	20010327
US 6894161	B2 Provisional	US 2001-279233P	20010327
AU 2002306912	A1	AU 2002-306912	20020327
US 20030013696	A1	US 2002-109141	20020327
US 6894161	B2	US 2002-109141	20020327

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2002306912	A1 Based on	WO 2002076453 A

PRIORITY APPLN. INFO: US 2001-279233P 20010327
US 2002-109141 20020327

INT. PATENT CLASSIF.:
MAIN: A61K031-409
IPC RECLASSIF.: A61K0041-00 [I,A]; A61K0041-00 [I,C]; C07D0487-00 [I,C]; C07D0487-22 [I,A]

BASIC ABSTRACT:

WO 2002076453 A1 UPAB: 20060118

NOVELTY - Photosensitizer compounds are new.

DETAILED DESCRIPTION - Photosensitizer compounds of formula (I), (II), (III) or (IV) are new.

R1 and R4 = a group of formula ; n = 0 - 6;

M = metal selected from Co, Ni(II), Cu(II), Zn(II), Fe(III), Sn, Ge, Si, Ga, Al, Mn(III), Gd(III), In or Tc; R2, R5 and R6 = H, lower alkyl, carboxylic acid ester (or carbalkoxy) group (2-6C), hydroxy, nitro, amino, sulfonyl, -CONR7CO-, lower alkyl carboxylic acid, its salt, amide, ester or acylhydrazone;

R7 = 6-10C aryl or 1-6C alkyl; R3 = H, hydroxy, nitro, amino, carboxylic acid ester (or carbalkoxy) group (2-6C), sulfonyl, 6-10C aryl, lower alkyl carboxylic acid, its salt, amide, ester or acylhydrazone. INDEPENDENT CLAIMS are included for the following:

(1) Method for conducting photodynamic therapy (PDT) (M1) involving contacting a target substrate with (I), (II), (III) or (IV) and irradiating the substrate with light containing a wavelength which activates the compound; (2) Method for photoactivating a photoreactive moiety (M2) involving irradiating the moiety with long wavelength (preferably 625 - 700 nm) light to produce a reactive intermediate capable of forming a crosslink with another molecule; (3) Method for derivatizing (M3) a prophyrin, chlorin, bacteriochlorin or isobacteriochlorin molecule involving contacting a prophyrin, chlorin, bacteriochlorin or isobacteriochlorin molecule containing a vinyl moiety with diazomethane to produce a porphhyrin, chlorin or bacteriochlorin molecule capable of forming a reactive intermediate upon irradiation with long wavelength light; and
(4) A pyrazoline containing porphyrin, chlorin, bacteriochlorin or isobacteriochlorin molecule produced by the method (M3).
ACTIVITY - Cytostatic; Virucide; Antiarteriosclerotic; Vasotropic.
MECHANISM OF ACTION - None given.
USE - Compounds (I), (II), (III) and (IV) are involved in photactivating a photoreactive moiety and for conducting PDT (claimed) for the treatment of various conditions, tissues, and cells of a subject; for the diagnosis or treatment of cancer, reduction of activated leukocytes, treatment of ocular disorders, treatment and prevention of neovasculature and angiogenesis, destruction of viruses and cells infected by it, treatment of the atherosclerotic plaques, the treatment of restenosis and others.
ADVANTAGE - The photoporphyrin pyrazolines provides susceptibility to eliminate nitrogen on electronic excitation and create a reactive intermediate that will crosslink cellular components. The Compounds provides reduction of the PDT side effects such as damage to unintended tissues. The concentrations of the compounds cannot vary over any arbitary range, provides convenient index that can be adjusted according to the relative potency of the compound used and an increase in intensity would permit a decrease in time of irradiation. TECHNOLOGY FOCUS:

ORGANIC CHEMISTRY - Preparation: No general preparation of compounds (I), (II), (III) or (IV) is given.

Preferred Components: The reactive intermediate is radical, carbene or nitrene. The radical is produced by photoactivation of a pyrazoline, acetophenone, benzophenone, anthraquinone, anthrone or anthrone-like heterocycles. The carbene is produced by photoactivation of a diazirine, 3-trifluoromethyl-3-phenyldiazirine, ketene or diphenylketene. The nitrene is produced by photoactivation of an azide, phenyl azide, 4-fluoro-3-nitrophenyl azide, benzoyl azide, p-methylbenzoyl, ethyl azidoformate, phenyl azidoformate, benzenesulfonyl azide, diphenyl phosphoryl azide, diethyl phosphoryl azide, diazomethane, diphenldiazomethane, diazoacetophenone, 1-trifluoromethyl-1-diazo-2-pentanone, tert-butyl diazoacetate, phenyl diazoacetate, or tert-butyl alpha diazoacetoacetate. The moiety extrudes molecular nitrogen upon photoactivation to produce the reactive intermediate. The moiety is covalently attached to an active agent (preferably photosensitizer, especially prophyrin, chlorin, bacteriochlorin or isobacteriochlorin).

Preferred Method: The light also crosslinks with the compound to the target substrate. The method (M1) further involves repeat irradiation of the substrate with light

absorbed by the compound.

EXTENSION ABSTRACT:

ADMINISTRATION - The photosensitize compounds are administered in a dosage of 0.05 - 1 (preferably 1 - 10) mg/kg parenterally (including intravenously, subcutaneously, intramuscularly, intrathecal, intraperitoneally), aerosol intranasally, intrapulmonary or topically. EXAMPLE - A stirred deoxytenated solution of the pyrazoline of methylpyropheophorbide in benzene (2.75x10-4 g/ml) was irradiated in front of a 672 nm LED panel for 14 hours. This layer chromatography revealed completion of the reaction and benzene was removed in vacuo. The residue was dissolved in dichloromethane and the crude compound was chromatographed on silica gel and fractions were pooled and evaporated to give cyclopropane derivative of methylpyropheophorbide (98.6%).

FILE SEGMENT: CPI; GMPI
MANUAL CODE: CPI: B05-A03A; B05-A03B; B05-B01B; B06-D18; B07-D08; B12-K04A1; B14-A02; B14-F01G; B14-F02F2; B14-F07; B14-N03

L25 ANSWER 10 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2001-182476 [18] WPIX
DOC. NO. CPI: C2001-054330 [18]
TITLE: Olefin polymerization catalyst comprises a group 6 metal and a ligand capable of forming electron donor bonds and at least one further single atom to
single atom bond to the metal
DERWENT CLASS: A17; E12
INVENTOR: BLOM R; SMITH K T; TILSET M
PATENT ASSIGNEE: (BORA-C) BOREALIS TECHNOLOGY OY; (MARS-I) MARSDEN J
C
COUNTRY COUNT: 92

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2000078826	A1	20001228	(200118)*	EN	33[0]	
AU 2000055494	A	20010109	(200122)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2000078826	A1	WO 2000-GB2393	20000619
AU 2000055494	A	AU 2000-55494	20000619

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2000055494	A Based on	WO 2000078826 A

PRIORITY APPLN. INFO: GB 1999-14200 19990617
INT. PATENT CLASSIF.:
IPC RECLASSIF.: C08F0010-00 [I,A]; C08F0010-00 [I,C]; C08F0004-00 [I,C]; C08F0004-69 [I,A]
BASIC ABSTRACT:

WO 2000078826 A1 UPAB: 20060116

NOVELTY - An olefin polymerization catalyst comprises at least one metal complex comprising a group 6 metal and a ligand capable of forming:

(a) at least two electron donor bonds and (b) at least one further single atom to single atom bond to the metal.

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for an olefin (co)polymerization process using the catalyst.

USE - Olefin (co)polymerization catalyst, especially for ethylene (claimed).

ADVANTAGE - The catalyst allows greater control over the properties of the resultant polymer. TECHNOLOGY FOCUS:

ORGANIC CHEMISTRY - Preferred Ligand: The ligand contains two or more nitrogen or phosphorus atoms or carbene groups capable of forming electron donor bonds with the metal. It also contain atom(s) capable of forming a covalent sigma or pi bond or a carbene:metal bond with the metal. The ligand is preferably tridentate. Any carbene groups present in the ligand are preferably heterocyclic with the skeletal structure (IIa) or (IIb), especially (IIc).

X = N or optionally substituted CH;

R7 = methyl, phenyl, naphthyl, 2,6-dimethylphenyl, 2,6-diisopropylphenyl, 2,6-di-tert.-butylphenyl, mesityl or ferrocenyl; and

Z' = as Z, or one is -LZY (where L is a bond or linker group) and the other is (optionally substituted) alkyl or a 5- or 6-membered heterocyclic or carbocyclic ring.

Preferred Metal Complex: The metal complex is of formula (I).

M = Cr, Mo or W;

Q = an (in)organic group;

m = 2 or 3;

Y = CH, N, carbene or a 5- or 6-membered carbocyclic or heterocyclic ring;

Z = -(CR12)n-NR2R3, -(CR12)n-PR2R3, -(CR12)n-AsR2R3, -(CR12)n-SbR2R3, -(CR12)p-CR1=R4 or carbene;

R1 = H or (optionally substituted) alkyl or 5- to 10-membered carbocyclic or heterocyclic, or two R1 groups together form a carbocycle;

R2, R3 = H or (optionally substituted) alkyl or 5- or 6-membered carbocyclic or heterocyclic, or together form a heterocycle;

R4 = H or (optionally substituted) alkyl or 5- or 6-membered carbocyclic or heterocyclic; and

n, p = 0-3.

Especially preferred complexes are of formula (Ia)-(Id).

A = N or P;

M = Cr;

R2, R3, R4 = H or 1-6C alkyl;

n = 1-3; and

X = chloride.

Preferred Catalyst: A cocatalyst (e.g. an alumoxane) and optionally another olefin polymerization catalyst (e.g. a metallocene) are present. The catalyst is supported on a solid support.

EXTENSION ABSTRACT:

DEFINITIONS - Preferred Definitions: - M = Cr; - Q = halogen; - Y = CH, N or an aromatic ring substituted by Z in the o,o'-

positions; - R1 = H; - R2, R3 = 1-6C alkyl; - m = 2; - n = 1; and - p = 0.

SPECIFIC COMPOUNDS - Complexes where the metal is chromium(III) and the ligand is one of 33 specified e.g. - 2,6-bis (dimethylaminomethyl)phenyl, - 2,5- bis(dimethylaminomethyl) cyclopentyl, - bis(2- dimethylaminoethyl)amide, - 2,6-bis (dimethylphosphinemethyl)phenyl, - 3-(1,5-dimethylphosphine)pentyl or - 2,6-bis(imino)pyridyl. - The preferred complex is (2,6-bis (dimethylaminomethyl)phenyl) chromium dichloride.

EXAMPLE - A THF solution of (2,6- bis(dimethylaminomethyl)phenyl) lithium was added dropwise to a THF solution of CrCl3(THF)3 and stirred for 2 hours. Workup gave a 50% yield of (2,6-bis (dimethylaminomethyl)phenyl) chromium dichloride. The complex was used with methyl alumoxane cocatalyst in the polymerization of ethylene (no results given),

FILE SEGMENT: CPI
MANUAL CODE: CPI: A02-A06; A02-A06C; A04-G01A; E05-L03A; E05-M; E05-N

L25 ANSWER 11 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1999-094819 [08] WPIX
DOC. NO. CPI: C1999-027770 [08]
DOC. NO. NON-CPI: N1999-068972 [08]
TITLE: Solid-phase method for modifying substrate with peptide, especially adhesion-promoting peptide - applied to medical devices, e.g. vascular grafts, uses peptide modified by photoreactive group for covalent attachment
DERWENT CLASS: B04; D16; D22; P32
INVENTOR: FIELDS G B; MOORADIAN D L
PATENT ASSIGNEE: (MINU-C) UNIV MINNESOTA
COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
US 5853744	A	19981229	(199908)*	EN	14[4]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 5853744 A		US 1996-699965	19960820

PRIORITY APPLN. INFO: US 1996-699965 19960820
INT. PATENT CLASSIF.:
IPC RECLASSIF.: A61L0027-00 [I,C]; A61L0027-34 [I,A]; A61L0027-50 [I,A]; C12N0005-00 [I,A]; C12N0005-00 [I,C]
BASIC ABSTRACT:

US 5853744 A UPAB: 20050520 A solid-phase method for modifying a substrate surface to include a biomolecule (I) comprises (a) providing an immobilised (I), comprising a peptide having (i) an Nα-terminus or (ii) an active site, by covalently attaching it to a support; (b) attaching a photoreactive crosslinking agent (II), having at least one photoreactive group, to the immobilised peptide, in (i) at the Nα-terminus or in (ii) to the peptide at an amino acid that does not form part of the active site; (c) removing the photoreactive analogue (Ia) of (I) from the support

and (d) attaching (Ia) to a solid surface by activating the photoreactive group.

USE - The method is particularly used to immobilise (I) on medical devices, specifically adhesion-promoting peptides on vascular grafts such that adhesion of cells to the device is improved. More generally a wide range of peptides can be deposited on blood oxygenators, pumps or sensors; tubing; stents; pacemaker leads; heart valves; catheters; artificial organs; or body implants generally.

ADVANTAGE - Bound (I) retains its native activity, specifically promotion of adhesion and spreading of vascular endothelial cells. The method ensures that (II) reacts with α-amino groups only (contrast use of soluble peptide where reaction may occur at ε-amino groups in the active site) and a large excess of (II) can be used to avoid wasting peptide.

DOCUMENTATION ABSTRACT:

US5853744

A solid-phase method for modifying a substrate surface to include a biomolecule (I) comprises (a) providing an immobilised (I), comprising a peptide having (i) an Nα-terminus or (ii) an active site, by covalently attaching it to a support; (b) attaching a photoreactive crosslinking agent (II), having at least one photoreactive group, to the immobilised peptide, in (i) at the Nα-terminus or in (ii) to the peptide at an amino acid that does not form part of the active site; (c) removing the photoreactive analogue (Ia) of (I) from the support and (d) attaching (Ia) to a solid surface by activating the photoreactive group.

USE

The method is particularly used to immobilise (I) on medical devices, specifically adhesion-promoting peptides on vascular grafts such that adhesion of cells to the device is improved. More generally a wide range of peptides can be deposited on blood oxygenators, pumps or sensors; tubing; stents; pacemaker leads; heart valves; catheters; artificial organs; or body implants generally.

ADVANTAGE

Bound (I) retains its native activity, specifically promotion of adhesion and spreading of vascular endothelial cells. The method ensures that (II) reacts with α-amino groups only (contrast use of soluble peptide where reaction may occur at ε-amino groups in the active site) and a large excess of (II) can be used to avoid wasting peptide.

WIDER DISCLOSURE

(II) is also an antibacterial, antimicrobial, antithrombotic, enzyme, nucleic acid or dye.

EXAMPLE

A reaction mixture contained SASD (50 mg); N-hydroxybenzotriazole (12.5 mg) and resin-bound (2) (0.0462 mmole). After 4 hours reaction, the mixture was filtered, the resin washed and the SASD-(2) product cleaved from the resin by

treatment
with 5% aqueous trifluoroacetic acid (5 ml) for 2 hours. A solution
(50 µl) of this product, labelled with iodine-125, in pH 7.4 phosphate buffer was added to bacteriological grade polystyrene (PS) wells or to polyethylene terephthalate (PT) discs, allowed to adsorb and irradiated with 355 nm radiation, at a distance of 3 cm for 1-15 minutes. The materials were washed, blocked with albumin, then tested for adhesion of RHE-1A endothelial cells by incubation for 1 hour at 37°C in a 5% carbon dioxide/air atmosphere. The material was washed again then adhered cells lysed and the amount of radioactivity incorporated was measured. The figure shows
that the number of cells that adhered to treated PS (black symbols)
increased in a time-dependent manner, reaching 67% after 90 min, but that PS treated with SASD only (white symbols) retained far fewer cells. Similar results were observed with PT discs.
PREFERRED MATERIALS
(II) is a heterobifunctional photoreactive crosslinking agent and (I) is particularly the fibronectin fragment WQPPRARI (2) which is especially synthesised on the support. The substrate is a biomaterial, e.g. metal, carbon,
ceramic, organ or tissue, wood, glass, or a wide variety of polymers. (II) is a compound that decomposes to generate a nitrene,
carbene or triplet oxygen, and also includes a chemically reactive group. Preferred (II) is sulphosuccinimidyl 2-(p-azidosalicylamido)ethyl-1,3'-dithiopropionate (SASD) having a photoreactive arylazide and chemically reactive ester group.
PREFERRED METHOD
(Ia) is attached by applying it to the substrate then exposing to ultra-violet radiation. Step (b) may include, after reaction with (II), removal of any protecting groups in (Ia).

FILE SEGMENT: CPI; GMPI
MANUAL CODE: CPI: B04-N04; B11-C04A; D05-H10; D09-C01; D09-C01B;
D09-C01C

L25 ANSWER 12 OF 12 WPIX COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1996-393878 [40] WPIX
DOC. NO. CPI: C1996-123996 [40]
TITLE: Hydrophobically modified matrix surface for bio-sensor etc. - with covalently bonded hydrocarbon chain obtd. by irradiating carbene or nitrene crosslinker
DERWENT CLASS: B04; D16; E14; J04
INVENTOR: STEIN T
PATENT ASSIGNEE: (PLAC-C) MAX PLANCK GES FOERDERUNG WISSENSCHAFTEN
COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
DE 4436173	C1	19960905	(199640)*	DE	7[0]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 4436173 C1		DE 1994-4436173	19941010

PRIORITY APPLN. INFO: DE 1994-4436173 19941010
INT. PATENT CLASSIF.:
IPC RECLASSIF.: C07K0017-00 [I,C]; C07K0017-10 [I,A]; G01N0033-543 [I,A]; G01N0033-543 [I,C]

BASIC ABSTRACT:

DE 4436173 C1 UPAB: 20050513 Hydrophobically modified matrix surface has covalently bonded 4-12C chain, or cycloaliphatic or aromatic system. The modification is produced by reaction with a photochemical crosslinker, obtd. by irradiating a carbene or nitrene.

Also claimed is the process for preparation of the surface.

USE - The matrix surface is used for the immobilisation of lipids or proteins, and/or for use as a biosensor (claimed).

ADVANTAGE - The lipids and proteins can be immobilised under favourable, mild conditions, that do not damage the activity or structure of the immobilised material. The prod. can be washed with detergent without loss.

DOCUMENTATION ABSTRACT:

DE4436173

Hydrophobically modified matrix surface has covalently bonded 4-12C chain, or cycloaliphatic or aromatic system. The modification is produced by reaction with a photochemical crosslinker, obtd. by irradiating a carbene or nitrene.

Also claimed is the process for preparation of the surface.

USE

The matrix surface is used for the immobilisation of lipids or proteins, and/or for use as a biosensor (claimed).

ADVANTAGE

The lipids and proteins can be immobilised under favourable, mild conditions, that do not damage the activity or structure of the immobilised material. The prod. can be washed with detergent without loss.

EXAMPLE

(a) Carboxymethyl dextran matrix chips (Pharmacia)were and optically normalised by standard method;

(b) the carboxy gps. were activated by a 7-minute pulse of a mixture of N'-3-dimethylaminopropyl)- N-ethylcarbodiimine HCl/(EDC)/N-hydroxysuccinimide (NHS) at fluid rate 5 µl/ml;

(c) reaction of the activated COOH gps. with a 7 minute pulse of a solution of one of the pref. crosslinkers (1) in a standard buffer (10-100 mM);

(d) rinsing the system with buffer containing 10 mM HEPES and 3.4 mM EDTA;

(e) immobilisation of the lipid-anchored cell adhesion molecules (CsA) in a 25 minute pulse at a concentration of 100 µg/ml in a 10 mM HEPES buffer (pH 7.4) containing 3.4 mM EDTA and 250 mM

NaCl;
(f) determn. of the CsA with anti-CsA antibody. (RMH)
PREFERRED CROSSLINKER
The crosslinker has the formula:
X(CH2)8Y (I),
or the structure of formula (II);
X = NH2, CHO, SH or OH;
Y = a gp. of formulae (a) or (b).
PREFERRED PRODUCT
The matrix is modified with hexylamine, heptylamine,
octylamine or nonylamine.
FILE SEGMENT: CPI
MANUAL CODE: CPI: B04-B01B; B04-C02C; B04-N04; B07-D01; B10-A16;
B12-K04A; D05-A01A; D05-A01C2; E07-D01; E10-A16B; J04-B01B

=> fil hcap
FILE 'HCAPLUS' ENTERED AT 11:51:44 ON 17 DEC 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 17 Dec 2007 VOL 147 ISS 26
FILE LAST UPDATED: 14 Dec 2007 (20071214/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil compend
FILE 'COMPENDEX' ENTERED AT 11:51:47 ON 17 DEC 2007

FILE LAST UPDATED: 17 DEC 2007 <20071217/UP>
FILE COVERS 1970 TO DATE.

<<< SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN THE BASIC INDEX >>>

=> d l35 iall hitstr 1-18

L35 ANSWER 1 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN
ACCESSION NUMBER: 2006(12):10665 COMPENDEX Full-text
TITLE: C-H oxidative addition of bisimidazolium salts to iridium and rhodium complexes, and N-heterocyclic carbene generation. A combined experimental and theoretical study.
AUTHOR: Viciano, Monica (Departamento de Quimica Inorganica y Organica Universitat Jaume I, 12080
Castellon, Spain); Poyatos, Macarena; Sanau, Mercedes; Peris, Eduardo; Rossin, Andrea; Ujaque, Gregori; Lledos, Agusti
SOURCE: Organometallics v 25 n 5 Feb 27 2006 2006.p 1120-1134
SOURCE: Organometallics v 25 n 5 Feb 27 2006 2006.p 1120-1134
CODEN: ORGND7 ISSN: 0276-7333
PUBLICATION YEAR: 2006
DOCUMENT TYPE: Journal
TREATMENT CODE: Bibliography; Experimental
LANGUAGE: English
ABSTRACT: A series of bis-N-heterocyclic carbenes of rhodium and iridium have been obtained and characterized. The formation of the M-C bond has been studied according to experimental and theoretical data, showing that two different mechanisms are operative for the first (single proton deprotonation of the bisimidazolium salt, or oxidative addition followed by deprotonation of the metal hydride) and second (oxidative addition of the second bisimidazolium C-H bond, yielding a NHC-IrIII-H species) metalation processes. In the case of complexes with long linkers Between the imidazolium rings, reductive elimination of HCl affords bisimidazolylidene complexes of IrI. According to the theoretical studies we concluded that thermodynamic parameters would determine the formation of the NHC-IrIII-H species, while IrI-NHC species would be kinetically favored in the case of complexes with long linkers between the azole rings. The crystal structures of a series of Ir-bis(NHC) complexes are described. $CPY 2006 American Chemical Society. 52 Refs.
CLASSIFICATION CODE: 801.4 Physical Chemistry; 547.1 Precious Metals;
931.3 Atomic and Molecular Physics; 802.2 Chemical Reactions; 641.1 Thermodynamics
CONTROLLED TERM: *Chemical bonds; Rhodium; Iridium; Thermodynamic properties; Protons; Oxidation
SUPPLEMENTARY TERM: C-H oxidative addition; Bisimidazolium salts; N-heterocyclic carbene generation
ELEMENT TERM: N; C*H; C-H; H*I*Ir; IrIII; Ir cp; cp; I cp; IrIII-H; Cl*H; HCl; H cp; Cl cp; I*Ir; IrI; C*H*I*Ir*N; NHC; N cp; C cp; IrI-NHC; Ir

L35 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:213901 HCAPLUS Full-text
DOCUMENT NUMBER: 145:162105
ENTRY DATE: Entered STN: 09 Mar 2006
TITLE: Photochemical fishing approaches for identifying
target proteins and elucidating the structure of
a ligand-binding region using carbene-

generating
photoreactive probes
AUTHOR(S): Sadakane, Yutaka; Hatanaka, Yasumaru
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kyushu University of Health and Welfare, 1714-1 Yoshino-cho, Nobeoka, 882-8508, Japan
SOURCE: Analytical Sciences (2006), 22(2), 209-218
CODEN: ANSCEN; ISSN: 0910-6340
PUBLISHER: Japan Society for Analytical Chemistry
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
CLASSIFICATION: 9-0 (Biochemical Methods)
ABSTRACT:
A review. Photoaffinity labeling enables the direct probing of a target protein through a covalent bond between a ligand and its binding protein, and even a complex formed by weak interactions can be isolated by the method. The photochem. fishing approach accelerates the throughput, isolating crosslinked complexes and analyzing the structure of the ligand binding site within the protein. We used carbene-generating phenyldiazirine for this approach because practical examns. had shown that the phenyldiazirine functioned as the powerful barb on the hook. Improving the synthetic pathways of the photoprobes and using chemoselective-integrated photoreactive units makes possible the easy and rapid preparation of carbene-generating photoreactive probes
including the derivs. in peptides, proteins, DNAs, and carbohydrates. This review also shows several recent impacts of photoaffinity labeling, including the in vivo preparation of photoreactive proteins in living cells.

SUPPL. TERM: review protein ligand binding region identification carbene generating probe
INDEX TERM: Bond
(covalent; photochem. fishing approaches for identifying target proteins and elucidating the
structure of a ligand-binding region using carbene-generating photoreactive probes)
INDEX TERM: Proteins
ROLE: PRP (Properties); RCT (Reactant); RACT (Reactant
or reagent)
(ligand-binding; photochem. fishing approaches for identifying target proteins and elucidating the structure of a ligand-binding region using carbene-generating photoreactive probes)
INDEX TERM: Enzyme functional sites
Molecular association
Photoaffinity labeling
(photochem. fishing approaches for identifying target proteins and elucidating the structure of a ligand-binding region using carbene-generating photoreactive probes)
INDEX TERM: Carbohydrates, uses
DNA
Peptides, uses
ROLE: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
(photochem. fishing approaches for identifying target proteins and elucidating the structure of a

ligand-binding region using carbene-generating photoreactive probes)

INDEX TERM: Carbenes (bitumen components)
ROLE: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(photochem. fishing approaches for identifying target proteins and elucidating the structure of a ligand-binding region using carbene-generating photoreactive probes)

INDEX TERM: Ligands
Proteins
ROLE: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(photochem. fishing approaches for identifying target proteins and elucidating the structure of a ligand-binding region using carbene-generating photoreactive probes)

INDEX TERM: 42270-91-7, Phenyldiazirine
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(photochem. fishing approaches for identifying target proteins and elucidating the structure of a ligand-binding region using carbene-generating photoreactive probes)

REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):
(1) Brunner, J; Annu Rev Biochem 1993, V62, P483 HCAPLUS
(2) Brunner, J; J Biol Chem 1980, V255, P3313 HCAPLUS
(3) Chehade, K; J Org Chem 2000, V65, P4949 HCAPLUS
(4) Chin, J; J Am Chem Soc 2002, V124, P9026 HCAPLUS
(5) Chin, J; Proc Natl Acad Sci USA 2002, V99, P11020 HCAPLUS
(6) Cleary, M; Proc Natl Acad Sci USA 1997, V94, P8450 HCAPLUS
(7) Dorman, G; Biochemistry 1994, V33, P5661 HCAPLUS
(8) Dorman, G; Tre Biotechnol 2000, V18, P64 HCAPLUS
(9) Drees, B; Curr Opin Chem Biol 1999, V3, P64 HCAPLUS
(10) Driessen, A; Nat Struct Biol 2001, V8, P492 HCAPLUS
(11) Egnaczyk, G; Biochemistry 2001, V40, P11706 HCAPLUS
(12) Escher, E; J Med Chem 1978, V21, P860 HCAPLUS
(13) Esher, E; FEBS Lett 1974, V46, P347
(14) Farrell, I; Nat Methods 2005, V2, P377 HCAPLUS
(15) Fischli, W; Helv Chim Acta 1976, V59, P878 HCAPLUS
(16) Fleming, S; Tetrahedron 1995, V51, P12479 HCAPLUS
(17) Forget, D; Mol Cell Biol 2004, V24, P1122 HCAPLUS
(18) Galardy, R; Nat New Biol 1973, V242, P127 HCAPLUS
(19) Gastinel, L; EMBO J 1999, V18, P3546 HCAPLUS
(20) Hashimoto, M; Chem Pharm Bull 1999, V47, P667 HCAPLUS
(21) Hashimoto, M; Heterocycles 1997, V46, P119

HCAPLUS
(22) Hatanaka, Y; Bioorg Med Chem Lett 2001, V11,
P411
HCAPLUS
(23) Hatanaka, Y; Chem Pharm Bull 1994, V42, P826
HCAPLUS
(24) Hatanaka, Y; Curr Top Med Chem 2002, V2, P271
HCAPLUS
(25) Hatanaka, Y; J Am Chem Soc 1998, V120, P453
HCAPLUS
(26) Hatanaka, Y; J Org Chem 1994, V59, P383 HCAPLUS
(27) Hatanaka, Y; J Org Chem 2000, V65, P5639 HCAPLUS
(28) High, S; J Biol Chem 1993, V268, P26745 HCAPLUS
(29) Hino, N; Nat Methods 2005, V2, P201 HCAPLUS
(30) Hixson, S; Biochemistry 1975, V14, P4251 HCAPLUS
(31) Hohsaka, T; Biochemistry 2001, V40, P11060
HCAPLUS
(32) Hohsaka, T; Curr Opin Chem Biol 2002, V6, P809
HCAPLUS
(33) Kaneda, M; Bioconjugate Chem 2003, V14, P849
HCAPLUS
(34) Kanoh, N; Angew Chem, Int Ed 2003, V42, P5584
HCAPLUS
(35) Kanoh, N; Angew Chem, Int Ed 2005, V44, P3559
HCAPLUS
(36) Karney, W; J Am Chem Soc 1997, V119, P3347
HCAPLUS
(37) Kauer, J; J Biol Chem 1986, V261, P10695 HCAPLUS
(38) Kempin, U; Heterocycles 1998, V49, P465 HCAPLUS
(39) Kenyon, G; Methods Enzymol 1977, V47, P407
HCAPLUS
(40) Lauc, G; Glycobiology 2000, V10, P357 HCAPLUS
(41) Lelievre, D; Tetrahedron Lett 1998, V39, P9675
HCAPLUS
(42) Lemieux, G; Tre Biotechnol 1998, V16, P506
HCAPLUS
(43) Li, Y; J Am Chem Soc 1988, V110, P8092 HCAPLUS
(44) Maliarik, M; J Biol Chem 1988, V263, P11274
HCAPLUS
(45) Mayer, A; Gene 1995, V153, P1 HCAPLUS
(46) Musier-Forsyth, K; Biochemistry 1994, V33, P773
HCAPLUS
(47) Nassal, M; J Am Chem Soc 1984, V106, P7540
HCAPLUS
(48) O'Neil, K; J Biol Chem 1989, V264, P14571
HCAPLUS
(49) Pandey, A; Nature 2000, V405, P837 HCAPLUS
(50) Pendergrast, P; Proc Natl Acad Sci USA 1992,
V89,
P10287 HCAPLUS
(51) Pruss, D; Science 1996, V274, P614 HCAPLUS
(52) Sadakane, Y; Chemical Genomics 2004, P199
HCAPLUS
(53) Sadakane, Y; Photomed Photobiol 2003, V24, P85
(54) Sadakane, Y; Photomed Photobiol 2004, V25, P35
(55) Sadakane, Y; Photomed Photobiol 2005, V26, P35
(56) Samuelson, J; Nature 2000, V406, P637 HCAPLUS
(57) Schmidt, T; J Mol Biol 1996, V255, P753 HCAPLUS
(58) Schwyzer, R; Helv Chim Acta 1971, V54, P1395
HCAPLUS

(59) Scotti, P; EMBO J 2000, V19, P542 HCAPLUS
(60) Sears, P; Science 2001, V291, P2344 HCAPLUS
(61) Sengupta, S; J Biol Chem 2001, V276, P12636 HCAPLUS
(62) Sengupta, S; Methods 1999, V19, P434 HCAPLUS
(63) Shih, L; Anal Biochem 1985, V144, P132 HCAPLUS
(64) Singh, A; J Biol Chem 1962, V237, P3006 MEDLINE
(65) Smith, R; J Am Chem Soc 1973, V95, P5072 HCAPLUS
(66) Suchanek, M; Nat Methods 2002, V2, P261
(67) Tan, Y; J Biol Chem 2003, V278, P36531 HCAPLUS
(68) Taranenko, M; Eur J Biochem 2003, V270, P2945 HCAPLUS
(69) Tate, J; Nucleic Acids Res 1998, V26, P1421 HCAPLUS
(70) Tazuke, S; J Polym Sci Polym Lett Ed 1978, V16, P497 HCAPLUS
(71) Tazuke, S; Makromol Chem 1978, V179, P2603 HCAPLUS
(72) Wang, L; Science 2001, V292, P498 HCAPLUS
(73) Weber, P; J Pept Res 1997, V49, P375 HCAPLUS
(74) Westerheide, S; Nucleic Acids Res 1999, V27, P1635 HCAPLUS
(75) Yamaguchi, T; Nucleic Acids Res 1997, V25, P2352 HCAPLUS
(76) Yang, J; J Biol Chem 1992, V267, P10393 HCAPLUS
(77) Yang, S; Proc Natl Acad Sci USA 1994, V91, P12183 HCAPLUS
(78) Zhu, H; Curr Opin Chem Biol 2003, V7, P55 HCAPLUS
(79) Zofall, M; Nucleic Acids Res 2000, V28, P4382 HCAPLUS

IT 42270-91-7, Phenyldiazirine
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. fishing approaches for identifying target proteins and elucidating the structure of a ligand-binding region
using carbene-generating photoreactive probes)
RN 42270-91-7 HCAPLUS
CN 3H-Diazirine, 3-phenyl- (CA INDEX NAME)

L35 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:493757 HCAPLUS Full-text
DOCUMENT NUMBER: 143:22656
ENTRY DATE: Entered STN: 10 Jun 2005
TITLE: Photolinker macromolecules, metallic substrates,
ligands modified with the linkers, and process of preparation
INVENTOR(S): Sigrist, Hans; Chai Gao, Hui; Soury-Lavergne, Isabelle

PATENT ASSIGNEE(S): C.S.E.M. Centre Suisse d'Electronique et de Microtechnique, Switz.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
INT. PATENT CLASSIF.:
MAIN: G01N033-543
CLASSIFICATION: 9-16 (Biochemical Methods)
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005052580	A1	20050609	WO 2004-CH704	
				200411
				23
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1563306	A1	20050817	EP 2004-797261	
				200411
				23
EP 1563306	B1	20070214		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR, IS, YU				
US 2007149775	A1	20070628	US 2006-580317	
				200605
				23
PRIORITY APPLN. INFO.:			EP 2003-405851	A
				200311
				28
			WO 2004-CH704	W
				200411
				23

PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2005052580	ICM	G01N033-543
	IPCI	G01N0033-543 [ICM,7]
	IPCR	G01N0033-543 [I,C*]; G01N0033-543 [I,A]
	ECLA	G01N033/543F

EP 1563306	IPCI	G01N0033-543 [I,C]; G01N0033-543 [I,A]
	IPCR	G01N0033-543 [I,C]; G01N0033-543 [I,A]
US 2007149775	IPCI	C07H0001-00 [I,A]
	NCL	536/123.100

ABSTRACT:
The invention relates to a photolinker macromol. comprising photoactivable groups and sulfur-containing groups, which is attached to a metallic substrate, and optionally covalently bonded to a ligand, and the use thereof in biosensor systems, microarrays, nanoparticles, nanoassemblies and microparticles useful in bioanalytics, or the pharmaceutical, or textile industry. Thus OptoDex S was synthesized starting from aminodextran and 3-(trifluoromethyl)-3-(m-isothiocyanophenyl)diazirine; the obtained OptoDex A was treated on a chromatog. column with sulfosuccinimidyl-6-[3'-(2-pyrimidylditihio)propionamido] hexanoate (LC sulfo SPDP). OptoDex S was chemisorbed onto gold surfaces; fluorophor (Cy5)-labeled riboflavin binding protein, Cy3-labeled BSU and non-labeled mouse Ig were photoimmobilized to the OptoDex S-gold surface. Vitamin B2 was determined by surface plasmon resonance using the photoimmobilized riboflavin binding protein surface.

SUPPL. TERM: photolinker macromol metallic substrate photoimmobilization microarray technol biosensor nanoparticle

INDEX TERM: Coupling reaction
(photochem.; photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

INDEX TERM: Immobilization, molecular or cellular
(photoimmobilization; photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

INDEX TERM: Biosensors
Chemisorption
Microarray technology
Microparticles
Nanoparticles
Surface plasmon resonance
Wavelength
(photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

INDEX TERM: Proteins
ROLE: ARG (Analytical reagent use); CPS (Chemical process); DEV (Device component use); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process); USES (Uses)
(riboflavin-binding, fluorophor-labeled; photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

INDEX TERM: 852920-70-8P, OptoDex S
ROLE: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(photolinker macromols., metallic substrates,

ligands modified with the linkers, and process of preparation)

INDEX TERM: 852920-72-0P, OptoDex SH
ROLE: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

INDEX TERM: 7429-90-5, Aluminum, uses 7440-05-3, Palladium, uses
7440-06-4, Platinum, uses 7440-22-4, Silver, uses
7440-50-8, Copper, uses 7440-57-5, Gold, uses
ROLE: DEV (Device component use); USES (Uses)
(photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

INDEX TERM: 9000-07-1, Carrageenan 9004-34-6, Cellulose, reactions 9004-54-0, Dextran, reactions 9005-25-8,
Starch, reactions 9005-32-7, Alginic acid
9012-36-6, Agarose 9044-05-7, Carboxymethyl dextran
26328-59-6 37293-51-9, Aminodextran 74261-65-7, p-Azidophenyl isothiocyanate 92944-71-3 96602-46-9
130973-94-3, 3-(Trifluoromethyl)-3-(m-isothiocyanophenyl)diazirine 176049-73-3,
4-(p-Azidosalicylamido)butylamine 852812-44-3
ROLE: DEV (Device component use); RCT (Reactant); RACT
(Reactant or reagent); USES (Uses)
(photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

INDEX TERM: 415697-73-3P, OptoDex A
ROLE: PRP (Properties); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

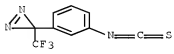
INDEX TERM: 852812-43-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Bergstroem; US 5242828 A 1993 HCAPLUS
(2) Chevolot, Y; BIOCONJUGATE CHEMISTRY 1999, V10(2), P169 HCAPLUS
(3) Gao, H; ANNUAL REPORT 2003 OF CENTRE SUISSE D'ELECTRONIQUE ET MICROTECHNIQUE,

http://www.csem.ch/corporate/Report2003/pdf/p71.pdf 2003, P71
(4) Nilsson, K; WO 9424561 A 1994 HCAPLUS
(5) Sigrist, H; OPTICAL ENGINEERING 1995, V34(8), P2339 HCAPLUS

IT 130973-94-3, 3-(Trifluoromethyl)-3-(m-isothiocyanophenyl)diazirine
RL: DEV (Device component use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(photolinker macromols., metallic substrates, ligands modified with the linkers, and process of preparation)
RN 130973-94-3 HCAPLUS
CN 3H-Diazirine, 3-(3-isothiocyanatophenyl)-3-(trifluoromethyl)- (CA INDEX NAME)



L35 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:654230 HCAPLUS Full-text
DOCUMENT NUMBER: 143:333472
ENTRY DATE: Entered STN: 27 Jul 2005
TITLE: Formation of Catalytic Metal-Molecule Contacts
AUTHOR(S): Tulevski, George S.; Myers, Matt B.; Hybertsen, Mark S.; Steigerwald, Michael L.; Nuckolls, Colin
CORPORATE SOURCE: Department of Chemistry and the Nanoscience Center, Columbia Univ., New York, NY, 10027, USA
SOURCE: Science (Washington, DC, United States) (2005), 309(5734), 591-594
CODEN: SCIEAS; ISSN: 0036-8075
PUBLISHER: American Association for the Advancement of Science
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 22, 35, 66, 73

ABSTRACT:
The authors describe a new strategy for the in situ growth of mol. wires predicated on the synthesis of a trifunctional primed contact formed from metal-C multiple bonds. The Ru-C π bond provides structural stability to the mol. linkages under ambient conditions, and d. functional calcns. indicate the formation of an efficient conduit for charge carriers to pass between the metal and the mol. Also, the metal-C π bond provides a chemical reactive site from which a conjugated mol. wire can be grown in situ through an olefin metathesis reaction.

SUPPL. TERM: ruthenium metal thin film reaction diazomethane; carbene ruthenium mol wire catalyst prepn olefin metathesis DFT
INDEX TERM: Density functional theory
(B3LYP; reaction of bromophenyldiazomethane with

ruthenium metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: Photoelectron spectra
(of ruthenium carbene mol. wire complex)

INDEX TERM: Metathesis catalysts
(olefin; reaction of bromophenyldiazomethane with ruthenium metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: Metathesis
(olefino; reaction of bromophenyldiazomethane with ruthenium metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: Molecular structure
(optimized; reaction of bromophenyldiazomethane with ruthenium metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: Electric contacts
Surface reaction
(reaction of bromophenyldiazomethane with ruthenium
metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: Carbene complexes
ROLE: PRP (Properties); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of bromophenyldiazomethane with ruthenium
metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: 821-07-8
ROLE: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(DFT calculated optimized geometries; reaction of bromophenyldiazomethane with ruthenium metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: 18107-18-1DP, reaction products with ruthenium thin film 73900-14-8DP, reaction products with ruthenium thin film
ROLE: PRP (Properties); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(IR and x-ray photoelectron spectra; reaction of bromophenyldiazomethane with ruthenium metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: 7440-18-8DP, Ruthenium, 4-bromophenylmethylidene,

trimethylsilylmethylidene, pentadienylidene, pentadienyl surface attached derivs.
ROLE: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(reaction of bromophenyldiazomethane with ruthenium
metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: 754-05-2, Vinyl trimethylsilane 7440-18-8, Ruthenium, reactions 18107-18-1, Trimethylsilyldiazomethane 73900-14-8, 4-Bromophenyldiazomethane
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of bromophenyldiazomethane with ruthenium
metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

INDEX TERM: 2039-82-9P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of bromophenyldiazomethane with ruthenium
metal thin film to give ruthenium carbene mol. wire as catalyst for surface-initiated olefin metathesis)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):
(1) Anon; The ABINIT code is a common project of the Universite Catholique de Louvain, Corning Incorporated, and other contributors, www.abinit.org
(2) Arnold, R; Langmuir 2001, V17, P4980 HCAPLUS
(3) Birchem, T; Surf Sci 1995, V334, PL701 HCAPLUS
(4) Combes, J; Langmuir 1999, V15, P7870 HCAPLUS
(5) Gagne, M; Organometallics 1992, V11, P3933 HCAPLUS
(6) George, P; J Am Chem Soc 1983, V105, P1393 HCAPLUS
(7) Gonze, X; Comp Mater Sci 2002, V25, P478
(8) Grubbs, R; The Handbook of Olefin Metathesis, ed 1 2003
(9) Gunia, M; J Phys Chem B 2004, V108, P14025 HCAPLUS
(10) Jacobi, K; Phys Status Solidi A 2000, V177, P37 HCAPLUS
(11) Kaga, Y; Surf Sci Spectra 1999, V6, P68 HCAPLUS
(12) Nitzan, A; Science 2003, V300, P1384 HCAPLUS
(13) Perdew, J; Phys Rev Lett 1996, V77, P3865 HCAPLUS
(14) Schrodinger LLC; Jaguar 5.0 1991-2003
(15) Siaj, M; J Am Chem Soc 2004, V126, P9514 HCAPLUS
(16) Siaj, M; Surf Sci 2005, V579, P1 HCAPLUS
(17) Umbach, E; Solid State Commun 1984, V51, P365

HCAPLUS
(18) Wasserman, S; Langmuir 1989, V5, P1074 HCAPLUS
(19) Wuffman, D; Synth Commun 1988, V18, P2349
(20) Zahidi, F; Nature 2001, V409, P1023
(21) Zhong, H; J Electron Mater 2001, V30, P1493
HCAPLUS

L35 ANSWER 5 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN
ACCESSION NUMBER: 2004(16):6731 COMPENDEX Full-text
TITLE: Reactivity Differences in the Syntheses of Chelating N-Heterocyclic Carbene Complexes of Rhodium Are Ascribed to Ligand Anisotropy.
AUTHOR: Mata, Jose A. (Chemistry Department Yale University, New Haven, CT 06520, United States);
Chianese, Anthony R.; Miecznikowski, John R.; Poyatos, Macarena; Peris, Eduardo; Faller, Jack W.; Crabtree, Robert H.
SOURCE: Organometallics v 23 n 6 Mar 15 2004 2004.p 1253-1263
SOURCE: Organometallics v 23 n 6 Mar 15 2004 2004.p 1253-1263
CODEN: ORGND7 ISSN: 0276-7333
PUBLICATION YEAR: 2004
DOCUMENT TYPE: Journal
TREATMENT CODE: Experimental
LANGUAGE: English
ABSTRACT: Chelating bis(imidazolium) salts having (CH2)n chains of different lengths (n = 1-4) linking the diazole rings show very large reactivity differences on metalation with [(cod)RhCl]2. Long linkers favor a square-planar Rh(I) product, while short linkers favor octahedral Rh(III). We ascribe the origin of the effect to the restricted rotation of the highly sterically anisotropic diazole rings and the different preferred orientations of these rings as n changes. Defining the x and y axes as the Rh-carbene bond directions, we find that with short linkers the diazole rings tend to be oriented close to the xy plane. This tends to favor Rh(III) because these complexes, [Rh (bis-carbene)I2(OAc)], have the lowest steric hindrance in the xy plane. With long linkers, the diazole rings tend to be aligned face to face along the +- z axis. This tends to favor Rh(I) because these complexes, [(cod)Rh(bis- carbene)]PF6, have the lowest steric hindrance along the +- z axis. Crystallographic studies are reported. Electrospray MS data provide evidence for strong metal- carbene binding. 53 Refs.
CLASSIFICATION CODE: 804.1 Organic Components; 802.2 Chemical Reactions; 931.1 Mechanics; 803 Chemical Agents;
801.4 Physical Chemistry; 931.2 Physical Properties of Gases, Liquids and Solids
CONTROLLED TERM: *Aromatic hydrocarbons; Anisotropy; Crystallography; Salts; Rotation; Additives; Chemical bonds; Rhodium compounds; Complexation; Synthesis (chemical); Chelation
SUPPLEMENTARY TERM: Transmetalation reactions; Ligands
ELEMENT TERM: Cl*Rh; RhCl]; Rh cp; cp; Cl cp; Rh; I; Ac*O; (OAc)]; O cp; Ac cp; N

L35 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:810443 HCAPLUS Full-text
ENTRY DATE: Entered STN: 05 Oct 2004
TITLE: Approaches to Metal-Functionalized Dendrimers Containing Platinum (II) and Palladium (II) Carbene Complexes
AUTHOR(S): Manne, Sudhakar; Slaughter, LeGrande M.
CORPORATE SOURCE: Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078, USA
SOURCE: Abstracts, 60th Southwest Regional Meeting of the American Chemical Society, Fort Worth, TX, United States, September 29-October 4 (2004), SEPT04-150. American Chemical Society: Washington, D. C.
CODEN: 69FVXC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
ABSTRACT:
Metal-functionalized dendrimers have been investigated primarily as potential catalytic materials; other potential applications include exploitation of photophys. properties of these dendrimer complexes. Such applications require metal complexes that are attached to the dendrimer via strong covalent bonds, and herein we describe efforts toward this goal utilizing robust metal-carbene bonds as linkers. Platinum (II) and Palladium (II) isocyanide complexes with 6-phenyl-2,2'-bipyridine as a tridentate ligand with isocyanides [CH3NC, tBuNC, and 2,6-MeC6H3NC] have been prepared and characterized. Procedures for attachment of these precursors to polypropyleneimine (PPI) dendrimers have been developed. The mode of attachment of the complexes is via nucleophilic attack of the primary amine end groups of the dendrimer at the isocyanide ligand of the metal complexes, forming a new carbene ligand which tethers the complex to the dendrimer. These new, unusual polymer supported metal-***carbene*** complexes could act as catalyst precursors or could possess useful luminescent properties, potentially leading to useful new materials.

L35 ANSWER 7 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN
ACCESSION NUMBER: 2003(6):1363 COMPENDEX Full-text
TITLE: A ruthenium(II)-porphyrin-carbene complex with a weakly bonded methanol ligand.
AUTHOR: Kawai, Masashi (Department of Chemistry School of Science Kitasato University, Kanagawa 228-8555, Japan); Yuge, Hidetaka; Ken, Takeshi
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications v 58 n 12 December 2002
2002.p m581-m582
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications v 58 n 12 December 2002
2002.p m581-m582
CODEN: ACSCEE ISSN: 0108-2701
PUBLICATION YEAR: 2002
DOCUMENT TYPE: Journal
TREATMENT CODE: Experimental
LANGUAGE: English
ABSTRACT: The title diphenylcarbene porphyrin complex (diphenyl-

carbenyl-kC) (methanol-kO)(5,10,15,20,- tetra-p-tolylporphy-rinato-k4N) ruthenium(II) methanol solvate, [Ru(C13H10)- (C48H36N 4)(CH4O)]* CH4O, has a six-coordinate Ru atom with a methanol molecule as the second axial ligand. The carbene fragment is slightly distorted from an ideal sp2 configuration, with a C(phenyl)-C(carbene)-C(phenyl) angle of 112.2 (3)deg . The Ru-C bond length of 1.845 (3) A is comparable with other carbene complexes. The two phenyl rings of the carbene ligand are perpendicular to the carbene plane. Methanol solvate molecules link the methanol ligands of adjacent porphyrin complexes via hydrogen bonds. 9 Refs.

CLASSIFICATION CODE: 804.1 Organic Components; 801.4 Physical Chemistry; 931.3 Atomic and Molecular Physics; 803 Chemical Agents; 802.3 Chemical Operations; 801.1 Chemistry (General)

CONTROLLED TERM: *Ruthenium compounds; Methanol; Catalysts; Molecular structure; Ultraviolet spectroscopy; Nuclear magnetic resonance spectroscopy; Crystallization; Chemical bonds

SUPPLEMENTARY TERM: Ruthenium porphyrin carbene; Cyclopropanation

ELEMENT TERM: O; N; C*H; C13H; C cp; cp; H cp; C*H*N; C48H36N;

N cp; Ru; C(phenyl)-C(carbene)-C(phenyl); C*Ru; Ru-C

L35 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:3446 HCAPLUS Full-text

DOCUMENT NUMBER: 138:333586

ENTRY DATE: Entered STN: 03 Jan 2003

TITLE: DNA duplexes containing photoactive derivatives of 2'-deoxyuridine as photocrosslinking probes for EcoRII DNA methyltransferase-substrate interaction

AUTHOR(S): Koudan, Elizaveta V.; Subach, Oksana M.; Korshunova, Galina A.; Romanova, Elena A.; Eritja, Ramon; Gromova, Elizaveta S.

CORPORATE SOURCE: Department of Chemistry, Belozersky Institute of Physico-Chemical Biology, Moscow State University, Moscow, 119992, Russia

SOURCE: Journal of Biomolecular Structure & Dynamics (2002), 20(3), 421-428
CODEN: JBSDD6; ISSN: 0739-1102

PUBLISHER: Adenine Press

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 7-5 (Enzymes)

ABSTRACT:

EcoRII DNA methyltransferase (M.EcoRII) recognizes the DNA sequence 5'...CC*T/AGG...3' and catalyzes the transfer of the Me group from S-adenosyl-L-methionine to the C5 position of the inner cytosine residue (C*). We obtained several DNA duplexes containing photoactive 5-iodo-2'-deoxyuridine (i5dU) or 5-[4-(3-(trifluoromethyl)-3H-diazirin-3-yl)phenyl]-2'-deoxyuridine (Tfmdp-dU) to characterize regions of M.EcoRII involved in DNA binding and to investigate the DNA double helix conformational changes that take place during methylation. The efficiencies of methylation, DNA binding affinities and M.EcoRII-DNA

photocrosslinking yields strongly depend on the type of modification and its location within the EcoRII recognition site. The data obtained agree
with the flipping of the target cytosine out of the DNA double helix for catalysis. To probe regions of M.EcoRII involved in DNA binding , covalent conjugates M.EcoRII-DNA were cleaved by cyanogen
bromide followed by anal. of the oligonucleotide-peptides obtained. DNA duplexes containing i5dU or Tfmdp-dU at the central position of the recognition site, or instead of the target cytosine were crosslinked to the Gly268-Met391 region of the EcoRII methylase. Amino acid residues from this region may take part both in substrate recognition and stabilization of the extrahelical target cytosine residue.

SUPPL. TERM: EcoRII methyltransferase photocrosslink DNA conformation
INDEX TERM: Conformational transition
Molecular association
(DNA containing photoactive 2'-deoxyuridine derivs.
permits anal. of M.EcoRII interactions with DNA and
conformational changes in DNA during methylation)
INDEX TERM: DNA
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(DNA containing photoactive 2'-deoxyuridine derivs.
permits anal. of M.EcoRII interactions with DNA and
conformational changes in DNA during methylation)
INDEX TERM: Molecular recognition
(photocrosslinking studies of M.EcoRII identify region which may be involved in DNA recognition and
stabilization of extrahelical cytosine target residue)
INDEX TERM: Enzyme functional sites
(substrate-binding; photocrosslinking studies of M.EcoRII identify region which may be involved in DNA recognition and stabilization of extrahelical cytosine target residue)
INDEX TERM: 80747-19-9, EcoRII DNA methyltransferase
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(DNA containing photoactive 2'-deoxyuridine derivs.
permits anal. of M.EcoRII interactions with DNA and
conformational changes in DNA during methylation)
INDEX TERM: 54-42-2, 5-Iodo-2'-deoxyuridine 210107-39-4
ROLE: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(DNA containing photoactive 2'-deoxyuridine derivs. permits anal. of M.EcoRII interactions with
DNA and conformational changes in DNA during methylation)
INDEX TERM: 71-30-7, Cytosine
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)

(photocrosslinking studies of M.EcoRII identify region which may be involved in DNA recognition and stabilization of extrahelical cytosine target residue)

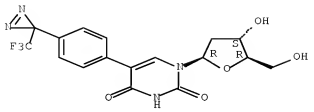
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):
(1) Babkina, O; Molecular Biology (Russ) 2000, V34, P913 HCAPLUS
(2) Brevnov, M; Nucleic Acids Res 1997, V25, P3302 HCAPLUS
(3) Brunner, J; J Biol Chem 1980, V255, P3313 HCAPLUS
(4) Connolly, B; Oligonucleotides and Analogues: A Practical Approach 1991
(5) Ferrer, E; Bioconjugate Chem 1997, V8, P757 HCAPLUS
(6) Friedman, S; Nucleic Acids Res 1992, V20, P3241 HCAPLUS
(7) Grachev, M; Eur J Biochem 1989, V180, P577 HCAPLUS
(8) Gritsenko, O; Nucleos Nucleot & Nucl Acids 2002, V21, P753 HCAPLUS
(9) Holz, B; J Biol Chem 1999, V274, P15066 HCAPLUS
(10) Jeltsch, A; J Mol Biol 1999, V285, P1121 HCAPLUS
(11) Klimasauskas, S; Cell 1994, V76, P357 MEDLINE
(12) Klimasauskas, S; Nucleic Acids Res 1995, V23, P1388 HCAPLUS
(13) Kossykh, V; FEBS Lett 1995, V370, P75 HCAPLUS
(14) Kumar, S; Nucleic Acids Res 1994, V22, P1 HCAPLUS
(15) Laemmli, U; Nature (London) 1970, V227, P680 HCAPLUS
(16) Meisenheimer, K; Crit Rev Biochem Mol Biol 1997, V32, P101 HCAPLUS
(17) Reinisch, K; J Mol Biol 1994, V238, P626 HCAPLUS
(18) Schroeder, S; Protein Eng 1997, V10, P1385 HCAPLUS
(19) Som, S; Nucleic Acids Res 1987, V15, P313 HCAPLUS
(20) Topin, A; Nucleotides and Nucleosides 1998, V17, P1163 HCAPLUS
(21) Vilkaitis, G; J Biol Chem 2000, V275, P38722 HCAPLUS
(22) Wong, D; Biochemistry 2000, V39, P15410 HCAPLUS
(23) Wu, J; J Biol Chem 1987, V262, P4778 HCAPLUS
(24) Wyszynski, M; Nucleic Acids Res 1993, V21, P295 HCAPLUS
(25) Yang, S; Nucleic Acids Res 1995, V23, P1380

IT 210107-39-4
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(DNA containing photoactive 2'-deoxyuridine derivs. permits anal. of M.EcoRII interactions with DNA and conformational changes in DNA during methylation)

RN 210107-39-4 HCAPLUS
CN Uridine, 2'-deoxy-5-[4-[3-(trifluoromethyl)-3H-diazirin-3-yl] phenyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L35 ANSWER 9 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN
ACCESSION NUMBER: 2006(50):5392 COMPENDEX Full-text
TITLE: Photoactive reagents for the covalent immobilization of polymer thin films.
AUTHOR: Yan, Mingdi (Department of Chemistry Portland State University, Portland, OR 97201)
SOURCE: Polymer News v 27 n 1 2002.p 6-12
SOURCE: Polymer News v 27 n 1 2002.p 6-12
CODEN: PLYNBU ISSN: 0032-3918
PUBLICATION YEAR: 2002
DOCUMENT TYPE: Journal
TREATMENT CODE: Bibliography; Theoretical
LANGUAGE: English
ABSTRACT: This review outlines the photochemical immobilization of polymer thin films by way of a covalently attached photochemically active reagent on solid substrates. The photochemical crosslinker has a functional group and a photoactive moiety. The functional group reacts with the solid substrate and covalently binds the light-sensitive group to the substrate. A polymer is then coated on the derivatized surface. UV irradiation generates the reactive intermediate from the photoactive group which then reacts with the neighboring polymer chains. The result is the covalent immobilization of a polymer thin film to the substrate. The method is versatile because the photochemistry is independent of the chemical natures of polymers to be immobilized. Most remarkably, it allows for the fabrication of patterned polymer thin films and microarrays, simply by using a photomask during the photochemical activation. $CPY 2002 OPA (Overseas Publishers Association) Amsterdam B.V. 63 Refs.
CLASSIFICATION CODE: 815.1 Polymeric Materials; 741.3 Optical Devices
and Systems; 802.2 Chemical Reactions; 801.4 Physical Chemistry; 741.1 Light. Optics; 804.1 Organic Compounds
CONTROLLED TERM: *Thin films; Optical materials; Crosslinking; Chemical bonds; Photochemical reactions; Aromatic compounds; Ketones; Polymers
SUPPLEMENTARY TERM: Microarrays; Photomask; Photochemical immobilization; Polymer thin films; Benzophenones; Aryidiazirines; Azides

L35 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:845782 HCAPLUS Full-text
DOCUMENT NUMBER: 137:47369
ENTRY DATE: Entered STN: 21 Nov 2001

TITLE: Immobilisation on polystyrene of diazirine derivatives of mono- and disaccharides: biological activities of modified surfaces

AUTHOR(S): Chevolot, Y.; Martins, J.; Milosevic, N.; Leonard, D.; Zeng, S.; Malissard, M.; Berger, E.
G.; Maier, P.; Mathieu, H. J.; Crout, D. H. G.; Sigrist, H.
CORPORATE SOURCE: Departement des Materiaux, LMCH, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.

SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(11), 2943-2953
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 33-4 (Carbohydrates)
Section cross-reference(s): 9, 36, 63
OTHER SOURCE(S): CASREACT 137:47369

ABSTRACT:
The potential of surface glycoengineering for biomaterials and biosensors originates from the importance of carbohydrate-protein interactions in biol. systems. The strategy employed here utilizes carbene generated by illumination of diazirine to achieve covalent bonding of carbohydrates. Here, we describe the synthesis of an aryl diazirine containing a disaccharide (lactose). Surface anal. techniques [XPS (XPS) and time of flight secondary ion mass spectroscopy (ToF-SIMS)] demonstrate its successful surface immobilization on polystyrene (PS). Results are compared to those previously obtained with an aryl diazirine containing a monosaccharide (galactose). The biol. activity of galactose- or lactose-modified PS samples is studied using rat hepatocytes, Allo A lectin and solid-phase semi-synthesis with α-2,6-sialyltransferase. Allo A shows some binding to galactose-modified PS but none to lactose-modified surfaces. Similar results are obtained with rat hepatocytes. In contrast, sialylation of lactose-modified PS is achieved but not with galactose-modified surfaces. The different responses indicate that the biol. activity depends not only on the carbohydrate per se but also on the structure and length of the spacer.

SUPPL. TERM: carbohydrate polystyrene prepn photoimmobilization surface analysis glycoengineering sialylation
INDEX TERM: Agglutinins and Lectins
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(A; preparation and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)
INDEX TERM: Sialylation
(preparation of lactoaryldiazirine attached to polystyrene and its enzymic sialylation for glycoengineering)
INDEX TERM: Glycation
Immobilization, molecular or cellular
Photochemistry

Surface analysis
(synthesis and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)

INDEX TERM: Carbohydrates, preparation
ROLE: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)

INDEX TERM: 222624-23-9DP, polystyrene-bound
331442-99-0DP, polystyrene-bound
ROLE: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)

INDEX TERM: 105-60-2, ε-Caprolactam, reactions 6291-42-5 79694-40-5 222624-23-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)

INDEX TERM: 17689-17-7P 331442-99-0P 438194-49-1P 438194-50-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)

INDEX TERM: 62-56-6, Thiourea, reactions
ROLE: RGT (Reagent); RACT (Reactant or reagent)
(preparation of)

INDEX TERM: 438232-10-1DP, polystyrene-bound
ROLE: BPN (Biosynthetic preparation); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of lactoaryldiazirine attached to polystyrene and its enzymic sialylation for glycoengineering)

INDEX TERM: 9075-81-4
ROLE: CAT (Catalyst use); USES (Uses)
(preparation of lactoaryldiazirine attached to polystyrene and its enzymic sialylation for glycoengineering)

INDEX TERM: 343614-02-8
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of lactoaryldiazirine attached to

polystyrene and its enzymic sialylation for glycoengineering)

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):

(1) Adachi, N; J Biomater Sci Polym Ed 1994, V6, P463 HCAPLUS
(2) Anon; Operator's Reference Manual Part No 625612 1992
(3) Ashwell, G; Annu Rev Biochem 1982, V51, P531 HCAPLUS
(4) Baenziger, J; J Biol Chem 1980, V255, P4607 HCAPLUS
(5) Baenziger, J; J Biol Chem 1980, V255, P4607 HCAPLUS
(6) Bernacki, R; Eur J Biochem V477, P58
(7) Biessen, E; Biochem J 1994, V229, P291
(8) Biessen, E; J Med Chem 1995, V38, P1538 HCAPLUS
(9) Bodanzky, M; Peptide Synthesis 1993
(10) Borenfreund, E; Toxicol In Vitro 1988, V2, P1 HCAPLUS
(11) Borenfreund, E; Toxicol Lett 1985, V24, P119 HCAPLUS
(12) Braun, J; J Biol Chem 1996, V271, P21160 HCAPLUS
(13) Buskas, T; Tetrahedron: Asymmetry 1994, V5, P2187 HCAPLUS
(14) Chevolot, Y; Bioconjugate Chem 1999, V10, P169 HCAPLUS
(15) Collioud, A; Bioconjugate Chem 1993, V4, P528 HCAPLUS
(16) Connolly, D; J Biol Chem 1982, V257, P939 HCAPLUS
(17) de la Torre, B; Peptide Protein Res 1990, V36, P86
(18) Elofsson, M; Tetrahedron 1991, P7613 HCAPLUS
(19) Franzreb, K; Surf Interface Anal 1995, V23, P641 HCAPLUS
(20) Gao, H; Biosens Bioelectron 1995, V10, P317 HCAPLUS
(21) Gao, H; Sens Actuator B 1997, V38-39, P38
(22) Hatanaka, K; Carbohyd Chem 1994, V13, P603 HCAPLUS
(23) Hermanson, G; Immobilized Affinity Ligand Techniques 1992, V1, P137
(24) Kawasaki, T; J Biol Chem 1976, V251, P12
(25) Lee, R; Biochemistry 1982, V21, P1045 HCAPLUS
(26) Lee, R; Biochemistry 1982, V21, P6292 HCAPLUS
(27) Lee, Y; Accounts Chem Res 1995, V28, P321 HCAPLUS
(28) Leonard, D; Surf Interface Anal 1998, V26, P783 HCAPLUS
(29) Leonard, D; Surf Interface Anal 1998, V26, P793 HCAPLUS
(30) Lopina, S; Biomaterials 1996, V17, P559 HCAPLUS
(31) Malissard, M; Glycoconjugate J 1999, V16, P125 HCAPLUS
(32) Massimi, M; Bioscience Rep 1996, V16, P477 HCAPLUS
(33) Milosevic, N; Eur J Pharmacol 1999, V368, P75

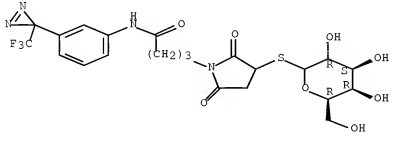
HCAPLUS
(34) Onyiriuka, E; Appl Spectrosc 1990, V44, P808 HCAPLUS
(35) Petrak, K; Adv Drug Deliv Rev 1994, V13, P211
(36) Rademacher, R; Annu Rev Biochem 1988, V57, P785
(37) Rademann, J; J Org Chem 1997, V62, P3650 HCAPLUS
(38) Rademann, J; Tetrahedron Lett 1996, V37, P3989 HCAPLUS
(39) Ratner, B; J Biomed Mater Res 1993, V27, P837 HCAPLUS
(40) Ruiz, L; Biomaterials 1998, V19, P987 HCAPLUS
(41) Saad, B; In Vitro Cell Dev Biol 1993, V29A, P32 MEDLINE
(42) Schueler, B; Microsc Microanal Microstruct 1992, V3, P119
(43) Schwartz, A; Annu Rev Immunol 1990, V8, P195 HCAPLUS
(44) Shimada, K; Biochim Biophys Acta 1997, V1326, P329 HCAPLUS
(45) Sigrist, H; Opt Eng 1995, V34, P2339 HCAPLUS
(46) Stockert, R; Targeted Diagnosis Ther 1991, V12, P441
(47) Varki, A; Glycobiology 1995, V3, P97
(48) Wortelboer, H; J Biochem Pharmacol 1990, V42, P381
(49) Yamada, K; Carbohydr Res 1998, V305, P443
(50) Yamashita, K; Method Enzymol 1989, V179, P331 HCAPLUS

IT 222624-23-9DP, polystyrene-bound 331442-99-0DP, polystyrene-bound
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)

RN 222624-23-9 HCAPLUS

CN 1-Pyrrolidinebutanamide, 3-(D-galactopyranosylthio)-2,5-dioxo-N-[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]- (CA INDEX NAME)

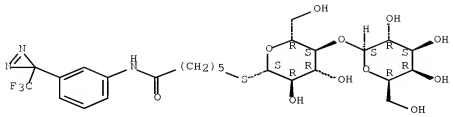
Absolute stereochemistry.



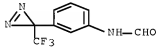
RN 331442-99-0 HCAPLUS

CN Hexanamide, 6-[(4-O-β-D-galactopyranosyl-β-D-glucopyranosyl)thio]-N-[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

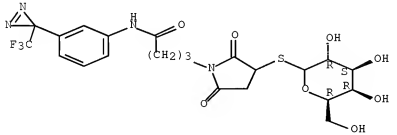


IT 79684-40-5 222624-23-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)
RN 79684-40-5 HCAPLUS
CN Formamide, N-[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]- (CA INDEX NAME)



RN 222624-23-9 HCAPLUS
CN 1-Pyrrolidinebutanamide, 3-(D-galactopyranosylthio)-2,5-dioxo-N-[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

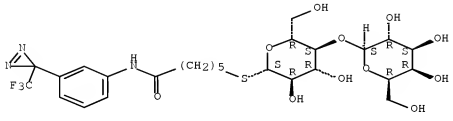


IT 331442-99-0P 438194-56-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and characterization of a photoactivatable glycoaryldiazirine and its attachment to polystyrene for surface glycoengineering)

RN 331442-99-0 HCAPLUS

CN Hexanamide, 6-[(4-O-β-D-galactopyranosyl-β-D-glucopyranosyl)thio]-N-[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]- (CA INDEX NAME)

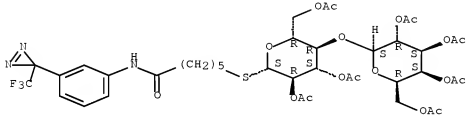
Absolute stereochemistry.



RN 438194-50-4 HCAPLUS

CN Hexanamide, 6-[(2,3,6-tri-O-acetyl-4-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-β-D-glucopyranosyl]thio]-N-[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.



L35 ANSWER 11 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN

ACCESSION NUMBER: 2001(56):1029 COMPENDEX Full-text

TITLE: Molecular magnetism via resonating valence bonds

for conjugated radicals and selected transition metal complexes.

AUTHOR: Klein, D.J. (Texas A and M University, Galveston, TX 77553-1675, United States); March, N.H.

MEETING TITLE: International Symposium on Atomic, Molecular and Condensed Matter Theory.

MEETING LOCATION: St.Augustine, FL, United States

MEETING DATE: 24 Feb 2001-02 Mar 2001

SOURCE: International Journal of Quantum Chemistry v 85 n 4-5 Nov 15 2001 2001.p 327-344

SOURCE: International Journal of Quantum Chemistry v 85 n 4-5 Nov 15 2001 2001.p 327-344
CODEN: IJQCB2 ISSN: 0020-7608

PUBLICATION YEAR: 2001
MEETING NUMBER: 58886
DOCUMENT TYPE: Conference Article
TREATMENT CODE: Experimental
LANGUAGE: English

ABSTRACT: Currently there is considerable interest in the nature of exchange interactions leading to unpaired electrons in molecular and cluster magnets. Here, the focus is largely at a qualitative level, via a novel "mean-field" resonance-theoretic view, to deal with exchange couplings, so as to allow unpaired electrons in either (or both of) the pi- and sigma-parts of a (largely organic) bipartite (or alternate) molecular network. The (quantitative) number and (qualitative) location of unpaired spins are dealt with by this simple approach, which also offers some (qualitative) information on the occurrence of low-lying higher-spin states. To illustrate the approach it is applied to a variety of systems where the spin sources are conjugated pi-network molecules and polymers, carbenes , variously defected graphites, and a few species involving transition metals, especially Cu. The discussion deals not only with traditional conjugated organics compounds but also with selected inorganic species. 134 Refs. CLASSIFICATION CODE: 708.4 Magnetic Materials; 804 Chemical Products Generally; 801.4 Physical Chemistry; 701.2 Magnetism: Basic Concepts and Phenomena; 931.1 Mechanics; 931.3 Atomic and Molecular Physics

CONTROLLED TERM: *Magnetic materials; Molecular dynamics; Magnetism; Resonance; Chemical bonds; Molecular structure; Electron energy levels; Transition metal compounds; Free radicals

SUPPLEMENTARY TERM: Conjugated radicals; Molecular magnetism; Resonating valence bonds; Exchange interactions; Cluster magnets; Molecular network; Polyradicals; Resonance theory

ELEMENT TERM: Cu

L35 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:795709 HCAPLUS Full-text
DOCUMENT NUMBER: 132:40580
ENTRY DATE: Entered STN: 17 Dec 1999
TITLE: Method for producing biocompatible surfaces
INVENTOR(S): Herbst, Franz; Kalatchev, Alexei
PATENT ASSIGNEE(S): Germany
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
INT. PATENT CLASSIF.: A61L027-00
CLASSIFICATION: 63-7 (Pharmaceuticals)
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964085	A1	19991216	WO 1998-EP8022	

199812

W: AU, BG, BR, CA, CZ, HU, ID, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, TR, UA, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AU 9918777 A 19991230 AU 1999-18777

199812

09

EP 1087799 A1 20010404 EP 1998-963549

199812

09

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI

JP 2002517285 T 20020618 JP 2000-553152

199812

09

PRIORITY APPLN. INFO.: WO 1998-EP3465 W

199806

09

WO 1998-EP8022 W

199812

09

PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9964085	IC	A61L027-00
	IPCI	A61L0027-00
	IPCR	A61L0029-00 [I,C*]; A61L0029-00 [I,A]; A61F0002-00 [N,C*]; A61F0002-00 [N,A]; A61L0027-00 [I,C*]; A61L0027-30 [I,A]; A61L0031-00 [I,C*]; A61L0031-00 [I,A]; A61L0031-08 [I,C*]; A61L0031-08 [I,A]; A61L0031-14 [I,C*]; A61L0031-16 [I,A]; A61L0033-00 [I,C*]; A61L0033-00 [I,A]
	ECLA	A61L027/30A; A61L031/08B2; A61L031/16; A61L033/00H2; A61L033/00H2F
AU 9918777	IPCI	A61L0027-00; A61L0031-00; A61L0033-00
	IPCR	A61L0029-00 [I,C*]; A61L0029-00 [I,A]; A61F0002-00 [N,C*]; A61F0002-00 [N,A]; A61L0027-00 [I,C*]; A61L0027-30 [I,A]; A61L0031-00 [I,C*]; A61L0031-00 [I,A]; A61L0031-08 [I,C*]; A61L0031-08 [I,A]; A61L0031-14 [I,C*]; A61L0031-16 [I,A]; A61L0033-00 [I,C*]; A61L0033-00 [I,A]
EP 1087799	IPCI	A61L0027-00; A61L0031-00; A61L0033-00
	IPCR	A61L0027-00 [I,C*]; A61L0027-00 [I,A]; A61L0031-00 [I,C*]; A61L0031-00 [I,A]; A61L0033-00 [I,C*]; A61L0033-00 [I,A]
JP 2002517285	IPCI	A61L0029-00; A61L0031-00; A61L0033-00
	IPCR	A61L0029-00 [I,C*]; A61L0029-00 [I,A]; A61F0002-00 [N,C*]; A61F0002-00 [N,A]; A61L0027-00 [I,C*]; A61L0027-30 [I,A]; A61L0031-00 [I,C*]; A61L0031-00 [I,A]; A61L0031-08 [I,C*]; A61L0031-08 [I,A];

A61L0031-14 [I,C*]; A61L0031-16 [I,A];
A61L0033-00 [I,C*]; A61L0033-00 [I,A]

ABSTRACT:
Medical objects such as implants and especially stents are endowed with a biocompatible diamondlike coating by use of a low-temperature plasma produced at reduced pressure in a gas or gas mixture containing ≥1 gaseous C compound and optionally a carrier gas by a combination of a radiofrequency source (which emits at a frequency in the MHz range) and an ultrasound source (which emits at a frequency in the kHz range). Plasma polymerization occurs at a gas pressure of 0.02-1 torr and an energy d. of 1-20 GJ/kg. A biomol., e.g. a natural product such as a glycosaminoglycan, is then covalently bound to the coating via a photoactive spacer layer of PEI; the biomol. first binds to the polyamine through ionic, hydrophobic , or H bonding, and covalent bonding is then effected by irradiation and generation of reactive carbenes. The biomol. preferably has an overall charge opposite to the polyamine; this makes it possible to work with very low concns. of the biomol., owing to a strong ionic concentration effect of the biomol. on the polyamine layer.
Thus, stents were placed vertically on a plate electrode in a reactor which was evacuated to <0.001 torr and then filled with Ar to a pressure of 0.04 torr. An Ar/CH4 (95:5) plasma was then generated at 0.04 torr, 13.46 MHz radiofrequency, and 20 kHz ultrasound frequency to produce a diamondlike layer 50 nm thick on the stents. The stents were then incubated in a solution of PEI coupled to photoactive 3-trifluoromethyl-3-(m-isothiocyanophenyl)diazirine, subsequently in a heparin solution, dried, and UV irradiated at 360 nm to bind the heparin covalently to PEI and the PEI to the diamondlike surface layer on the stents.

SUPPL. TERM: prosthesis surface biocompatibility plasma deposition PEI; heparin immobilization diamondlike coating stent
INDEX TERM: Noble gases, uses
ROLE: NUU (Other use, unclassified); USES (Uses)
(carriers; method for producing biocompatible surfaces)
INDEX TERM: Diamond-type crystals
(coatings; method for producing biocompatible surfaces)
INDEX TERM: Coating materials
(diamond-like; method for producing biocompatible surfaces)
INDEX TERM: Hydrocarbons, biological studies
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(fluoro; method for producing biocompatible surfaces)
INDEX TERM: Hydrocarbons, biological studies
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP

(Physical, engineering or chemical process); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(halo; method for producing biocompatible surfaces)

INDEX TERM: Plasma
(low-pressure; method for producing biocompatible surfaces)

INDEX TERM: Biochemical molecules
Biocompatibility
Cold plasma
Coupling agents
Medical goods
Radio wave
Sound and Ultrasound
Surface
(method for producing biocompatible surfaces)

INDEX TERM: Carbohydrates, biological studies
Glycosaminoglycans, biological studies
Hydrocarbons, biological studies
Organic compounds, biological studies
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(method for producing biocompatible surfaces)

INDEX TERM: Polymerization
Vapor deposition process
(plasma; method for producing biocompatible surfaces)

INDEX TERM: Medical goods
(stents; method for producing biocompatible surfaces)

INDEX TERM: 7440-37-1, Argon, uses
ROLE: NUU (Other use, unclassified); USES (Uses)
(carrier; method for producing biocompatible surfaces)

INDEX TERM: 130973-94-3, 3-Trifluoromethyl-3-(m-isothiocyanophenyl)diazirine
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(linker modified with; method for producing biocompatible surfaces)

INDEX TERM: 9002-98-6, PEI
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(linker; method for producing biocompatible surfaces)

INDEX TERM: 74-82-8, Methane, biological studies 9005-49-6, Heparin, biological studies 187888-07-9, Endostatin
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(method for producing biocompatible surfaces)

INDEX TERM: 86090-08-6, Angiostatin
ROLE: BAC (Biological activity or effector, except

adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(method for producing biocompatible surfaces)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):
(1) Biogold Inc; WO 8911919 A 1989 HCAPLUS
(2) Eastmond, G; Comprehensive Polymer Science 1989, V4
(3) Franke, R; DE 19630682 A 1997 HCAPLUS
(4) Franks, J; GB 2287473 A 1995 HCAPLUS
(5) Kao Corp; JP 08049077 A 1996 HCAPLUS
(6) NGK Spark Plug Co Ltd; JP 01270596 A 1989 HCAPLUS
(7) Narayanan, P; US 5132108 A 1992 HCAPLUS
(8) Sanyo Electric Co Ltd; JP 63072110 A 1988
(9) Talison Research; WO 9810116 A 1998 HCAPLUS
(10) Yoneda, M; US 5277740 A 1994 HCAPLUS
(11) Yuan, S; Journal of Applied Biomaterials 1995, V6(4), P259 HCAPLUS

L35 ANSWER 13 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN

ACCESSION NUMBER: 2000(26):3417 COMPENDEX Full-text

TITLE: Use of dextran as an intermediate layer: A new approach towards SAW based biosensors.

AUTHOR: Barie, N. (Inst fuer Instrumentelle Analytik, Karlsruhe, Ger); Rapp, M.; Sigrist, H.

SOURCE: Proceedings of the Annual IEEE International Frequency Control Symposium v 2 1999.p 997-1000

SOURCE: Proceedings of the Annual IEEE International Frequency Control Symposium v 2 1999.p 997-1000
CODEN: PAFSDB ISSN: 0161-6404

PUBLICATION YEAR: 1999

DOCUMENT TYPE: Journal

TREATMENT CODE: Experimental

LANGUAGE: English

ABSTRACT: We present a new method for covalent binding of dextran as an intermediate layer on surface acoustic wave (SAW) devices.The SAW devices were originally developed for use in modern telecommunications and are thus available as series products at low costs.For biosensing applications these devices must be coated with a shielding layer to prevent corrosion effects of the aluminum structures in aqueous media.Thin films of polyimide and parylene, respectively, showed good shielding properties and were used as a base for further immobilization.Dextran immobilization dextran to the polymer coated surfaces is achieved by a photoimmobilization process.A aryldiazirine-functionalized protein (T-BSA) serves as a mulifunctional light-activated linking agent (photolinker polymer). Dextran and the photolinker are mixed and photobonded to the sensor surface.Immobilization of proteins to the dextran layer via carbodiimide chemistry is exemplary demonstrated with anti-urease antibodies and the feasibility of specific immunosensing is investigated using SAW sensors connected to a fluid handling system.(Author abstract) 8 Refs.

CLASSIFICATION CODE: 461.9.1 Immunology; 801 Chemistry; 462.1 Biomedical Equipment (General); 752.1 Acoustic Devices; 804.1 Organic Components; 815.1.1 Organic Polymers

CONTROLLED TERM: *Immunosensors; Crosslinking; Corrosion prevention; Plastic films; Thin films; Polyimides; Enzyme immobilization; Proteins;

Acoustic surface wave devices; Polysaccharides
SUPPLEMENTARY TERM: Dextran; Parylene; Photoimmobilization processes; Photolinker polymers
ELEMENT TERM: T

L35 ANSWER 14 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN
ACCESSION NUMBER: 1999(4):3391 COMPENDEX Full-text
TITLE: Covalent photolinker-mediated immobilization of an intermediate dextran layer to polymer-coated surfaces for biosensing applications.
AUTHOR: Barie, N. (Forschungzentrum Karlsruhe GmbH, Karlsruhe, Ger); Rapp, M.; Sigrist, H.; Ache, H.J.
MEETING TITLE: Proceedings of the 1998 5th World Congress on Biosensors.
MEETING LOCATION: Berlin, Ger
MEETING DATE: 03 Jun 1998-05 Jun 1998
SOURCE: Biosensors & Bioelectronics v 13 n 7-8 Oct 1 1998.p 855-860
SOURCE: Biosensors & Bioelectronics v 13 n 7-8 Oct 1 1998.p 855-860
CODEN: BBIOE4 ISSN: 0956-5663
PUBLICATION YEAR: 1998
MEETING NUMBER: 49284
DOCUMENT TYPE: Journal
TREATMENT CODE: General Review
LANGUAGE: English
ABSTRACT: A new method is presented for the covalent binding of dextran as an intermediate layer on surface acoustic wave (SAW) devices.For biosensing applications in aqueous media commercially available SAW devices require surface passivation to prevent corrosion of the aluminum device structures in electrolytes.Thin films of polyimide and parylene revealed exceptional passivation properties.They were used as a base for dextran immobilization.Covalent binding of dextran to polymer-coated surfaces was achieved by photoimmobilization. Aryldiazirine-functionalized bovine serum albumin served as the multifunctional light-activable linking agent (photolinker polymer).Dextran and photolinker polymer were mixed and photobonded to sensor surfaces.Essential photoimmobilization parameters were optimized.The binding of proteins to dextran applying carbodiimide chemistries was exemplified with antiurease antibodies and the feasibility of specific immunosensing was investigated on SAW sensors connected to a fluid handling system. (Author abstract) 23 Refs.
CLASSIFICATION CODE: 461.9.1 Immunology; 815.1.1 Organic Polymers; 804.1 Organic Components; 539.2.1 Protection Methods; 539.2 Corrosion Protection; 817.1 Plastics Products
CONTROLLED TERM: *Immunosensors; Photochemical reactions; Passivation; Corrosion prevention; Plastic films; Polyimides; Plastic coatings; Antibodies; Polysaccharides; Acoustic surface wave devices
SUPPLEMENTARY TERM: Dextran; Photoimmobilization; Parylene; Photolinker polymers; Carbodiimide; Bovine serum albumin

L35 ANSWER 15 OF 18 COMPENDEX COPYRIGHT 2007 EEI on STN
ACCESSION NUMBER: 1997(37):5977 COMPENDEX Full-text
TITLE: Bioengineering of silicon nitride.

AUTHOR: Gao, Hui (CSEM Cent Suisse d'Electronique et de Microtechnique SA, Neuchatel, Switz); Luginbuhl, Reto; Sigrist, Hans
MEETING TITLE: Proceedings of the 1996 3rd European Conference on Optical Chemical Sensors and Biosensors, EUROPT(R)ODE III.Part 1 (of 2).
MEETING LOCATION: Zurich, Switz
MEETING DATE: 31 Mar 1996-03 Apr 1996
SOURCE: Sensors and Actuators, B: Chemical v B38 n 1-3 pt 1 Jan-Feb 1997.p 38-41
SOURCE: Sensors and Actuators, B: Chemical v B38 n 1-3 pt 1 Jan-Feb 1997.p 38-41
CODEN: SABCEB ISSN: 0925-4005
PUBLICATION YEAR: 1997
MEETING NUMBER: 46635
DOCUMENT TYPE: Journal
TREATMENT CODE: Experimental
LANGUAGE: English
ABSTRACT: Selective functionalization of silicon nitride with biomolecules by light-dependent processes has been investigated.Aryldiazirin -based photoimmobilization procedures are used to achieve covalent biomolecule binding.Experimentally facile processes applied include the following steps: (i) adsorptive coating of the surface with photolabel-bearing reagents or photolabel-functionalized biomolecules; (ii) exposure of the coated surface to activating light (350 nm); and (iii) removal of excess reagent or functionalized biomolecule.The extent of photoreagent binding to silicon nitride depends on the time of light exposure as well as on the amount of photoreagent applied to the surface.Streptavidin is immobilized by photolinker polymer-mediated procedures, and antibody-derived F(ab prime) fragments are covalently immobilized on silicon nitride (45-50 fmol mm minus 2) with a low-molecular -weight crosslinker.Biomolecule binding is monitored by fluorescein-labelled ligand binding and by tracing radiolabelled proteins, respectively.Photoimmobilized streptavidin retains ligand binding activity, and immunoreagents remain biologically active.Mask-assisted photopatterning on silicon nitride is achieved and patterned structures are resolved by atomic force microscopic imaging of photobonded diazirin-derivatized bovine serum albumin.(Author abstract) 11 Refs. CLASSIFICATION CODE: 804.2 Inorganic Components; 461.1 Biomedical Engineering; 461.8 Biotechnology; 801.2 Biochemistry; 804.1 Organic Components; 741.3 Optical Devices and Systems
CONTROLLED TERM: *Silicon nitride; Biomedical engineering; Enzyme immobilization; Atomic force microscopy; Photochemical reactions; Proteins
SUPPLEMENTARY TERM: Photoimmobilization; Aryldiazirin

L35 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:607633 HCAPLUS Full-text
DOCUMENT NUMBER: 126:70260
ENTRY DATE: Entered STN: 12 Oct 1996
TITLE: Synthesis and characterization of a photoactivatable analog of corticotropin-releasing factor for specific receptor labeling
AUTHOR(S): Ruehmann, Andreas; Koepke, Andreas K. E.; Dautzenberg, Frank M.; Spiess, Joachim
CORPORATE SOURCE: Department Molecular Neuroendocrinology, Max

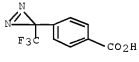
Planck Institute Experimental Medicine,
Goettingen, D-37075, Germany
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1996), 93(20), 10609-10613
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 2-1 (Mammalian Hormones)
Section cross-reference(s): 34

ABSTRACT:
A novel photoactivatable analog of ovine ACTH-releasing factor (ovine photoCRF) has been synthesized and characterized. A diazirine group, the 4-(1-azi-2,2,2-trifluoroethyl)benzoyl residue, was covalently bound to the amino terminus of ovine CRF (oCRF), which was N-terminally extended by a tyrosyl residue for radioactive labeling with 125I. Under mild conditions, photolysis yielded highly reactive carbenes, responsible for the formation of covalent bonds to the CRF receptor.
Ovine photoCRF was shown to bind to the high-affinity site of the CRF receptor with a similar Ed value as oCRF. When radioactively iodinated ovine photoCRF (ovine 125I-photoCRF) was covalently linked to rat CRF receptor, type 1 (rCRFR1), permanently transfected into human embryonic kidney (HEK) 293 cells, a highly glycosylated 75-kDa protein was identified with SDS/PAGE. The specificity of ovine 125I-photoCRF was demonstrated by the finding that this analog could be displaced from the receptor by oCRF, but not other unrelated peptides such as vasoactive intestinal peptide. The observed size of the 75-kDa cross-link was in agreement with the mol. weight reported earlier for native CRFR1 from rat
brain. Deglycosylation of the 75-kDa cross-link with peptide:N-glycosidase (PNGase) yielded a 46-kDa protein, in agreement with the mol. weight estimated from cDNA coding for rat CRFR1. The developed
CRF analog, photoCRF, is expected to facilitate future biochem. and physiol. anal. of CRF receptors and, by analogous strategies, of other peptide receptors.

SUPPL. TERM: photoactivatable CRF receptor labeling
INDEX TERM: Photoaffinity labeling
(CRF photoactivatable analog synthesis and characterization for specific receptor labeling)
INDEX TERM: Corticotropin releasing factor receptors
ROLE: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)
(type I; CRF photoactivatable analog synthesis and characterization for specific receptor labeling)
INDEX TERM: 103146-81-8DP, iodo derivs., iodine-125 labeled
ROLE: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL
(Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(CRF photoactivatable analog synthesis and characterization for specific receptor labeling)

INDEX TERM: 9015-71-8, ACTH-releasing factor
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(CRF photoactivatable analog synthesis and characterization for specific receptor labeling)
INDEX TERM: 85559-46-2P 183146-81-8P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(CRF photoactivatable analog synthesis and characterization for specific receptor labeling)
INDEX TERM: 873-75-6, 4-Bromobenzyl alcohol
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(bromobenzyl alc. in CRF photoactivatable analog synthesis)
IT 183146-81-8DP, iodo derivs., iodine-125 labeled
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(CRF photoactivatable analog synthesis and characterization for specific receptor labeling)
RN 183146-81-8 HCAPLUS
CN Corticotropin-releasing factor (sheep), N-[N-[4-[3-(trifluoromethyl)-
3H-diazirin-3-yl]benzoyl]-L-tyrosyl]-41-L-alanine- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT 85559-46-2P 183146-81-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(CRF photoactivatable analog synthesis and characterization for specific receptor labeling)
RN 85559-46-2 HCAPLUS
CN Benzoic acid, 4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)



RN 183146-81-8 HCAPLUS
CN Corticotropin-releasing factor (sheep), N-[N-[4-[3-(trifluoromethyl)-
3H-diazirin-3-yl]benzoyl]-L-tyrosyl]-41-L-alanine- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

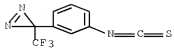
L35 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:637616 HCAPLUS Full-text
DOCUMENT NUMBER: 123:78951
ENTRY DATE: Entered STN: 24 Jun 1995

TITLE: Photochemical linkage of antibodies to silicon chips
AUTHOR(S): Sundarababu, Gajendran; Gao, Hui; Sigrist, Hans
CORPORATE SOURCE: Inst. Biochemistry, Univ. Bern, Bern, CH-3012, Switz.
SOURCE: Photochemistry and Photobiology (1995), 61(6), 540-4
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 9-16 (Biochemical Methods)
Section cross-reference(s): 15

ABSTRACT:
Antibodies and antigen-binding fragments thereof were photochem. immobilized on surface-modified silicon chips of 5 + 5 mm size. Silicon surface-grafted diazirines and benzophenones formed ***covalent*** bonds with the immunoreagents on light activation. Photolithog. immobilization of monoclonal antibodies in aqueous media was achieved on silicon chips by activating surface-grafted benzophenones. The presence of bovine serum albumin during irradiation reduced nonspecific adsorption of the immunoreagents and retained the immunoreactivity of the photoimmobilized mols.

SUPPL. TERM: antibody photochem immobilization silicon chip
INDEX TERM: Acetylation
Immobilization, biochemical
Semiconductor devices
(photochem. linkage of antibodies to silicon chips)
INDEX TERM: Antibodies
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(monoclonal, photochem. linkage of antibodies to silicon chips)
INDEX TERM: Lithography
(photo-, photochem. linkage of antibodies to silicon chips)
INDEX TERM: 919-30-2D, reaction products with silicon chips
7440-21-3, Silicon, reactions 26328-59-6D, reaction products with aminopropylated silicon chips
130973-94-3D, reaction products with aminopropylated silicon chips
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(photochem. linkage of antibodies to silicon chips)

IT 130973-94-3D, reaction products with aminopropylated silicon chips
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. linkage of antibodies to silicon chips)
RN 130973-94-3 HCAPLUS
CN 3H-Diazirine, 3-(3-isothiocyanatophenyl)-3-(trifluoromethyl)- (CA INDEX NAME)



L35 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:118049 HCAPLUS Full-text
DOCUMENT NUMBER: 114:118049
ENTRY DATE: Entered STN: 06 Apr 1991
TITLE: Philicity of amino acid side-chains for photogenerated carbenes
AUTHOR(S): Sigrist, Hans; Muehlemann, Marc; Dolder, Max
CORPORATE SOURCE: Inst. Biochem., Univ. Berne, Berne, CH-3012, Switz.
SOURCE: Journal of Photochemistry and Photobiology, B: Biology (1990), 7(2-4), 277-87
CODEN: JPPBEG; ISSN: 1011-1344
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 9-15 (Biochemical Methods)
Section cross-reference(s): 6

ABSTRACT:
The selectivity of a diazirine-photogenerated carbene towards amino acid side-chains was investigated by analyzing amino acid retention
following photocoupling with an immobilized carbene precursor. The heterobifunctional photocross-linker 3-(trifluoromethyl)-3-(m-isothiocyanophenyl)diazirine was synthesized and coupled to ***fiber*** glass. Photoinduced amino acid binding to the solid support was analyzed. The immobilized diazirine-photogenerated ***carbene*** preferentially binds to cysteine and aromatic amino acids.
Amino acids carrying sulfur or oxygen as side-chain heteroatoms are, in general, more carbene-philic than amino acids with aliphatic side-chains. Marginal carbene insertion is obtained with glycine. On the basis of the empirically determined photocoupling capacities
of the applied amino acids, a carbene philicity scale has been established. For homologous amino acids, carbene selectivity partly correlates with their hydrophobicity and the number of chem. bonds. Consequences of this distinct binding capacity are discussed with respect to photoselective protein modification.

SUPPL. TERM: amino acid philicity photogeneration carbene ; protein modification light
INDEX TERM: Light, chemical and physical effects
(in protein modification)
INDEX TERM: Proteins, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(modification of, photoselective)
INDEX TERM: Bond
(number of, of amino acids, carbene selectivity in relation to)
INDEX TERM: Hydrophobicity
(of amino acids, carbene philicity in

relation to)
INDEX TERM: Amino acids, properties
ROLE: PRP (Properties)
(philicity of, for photogenerated carbenes
)
INDEX TERM: Glass fibers, uses and miscellaneous
ROLE: USES (Uses)
(trifluoromethylisothiocyanophenyldiazirine
immobilization on)
INDEX TERM: Amino acids, properties
ROLE: PRP (Properties)
(aryl, philicity of, for photogenerated
carbenes)
INDEX TERM: 7732-18-5
ROLE: ANST (Analytical study)
(hydrophobicity, of amino acids, carbene
philicity in relation to)
INDEX TERM: 52-90-4, Cysteine, biological studies 56-40-6,
Glycine, biological studies 56-41-7, Alanine,
biological studies 56-45-1, Serine, biological
studies 56-84-8, Aspartic acid, biological studies
56-85-9, Glutamine, biological studies 56-86-0,
L-Glutamic acid, biological studies 56-87-1,
Lysine,
biological studies 60-18-4, Tyrosine, biological
studies 61-90-5, L-Leucine, biological studies
63-68-3, Methionine, biological studies 63-91-2,
Phenylalanine, biological studies 70-47-3,
Asparagine, biological studies 71-00-1, Histidine,
biological studies 72-18-4, Valine, biological
studies 72-19-5, Threonine, biological studies
73-22-3, Tryptophan, biological studies 73-32-5,
Isoleucine, biological studies 74-79-3, Arginine,
biological studies 147-85-3, L-Proline, biological
studies
ROLE: BIOL (Biological study)
(philicity of, for photogenerated carbenes
)
INDEX TERM: 130973-94-3P
ROLE: PREP (Preparation)
(preparation and coupling to fiber glass)
INDEX TERM: 79684-40-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and deformylation of)
INDEX TERM: 130973-96-5
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thiophosgene)
INDEX TERM: 463-71-8, Thiophosgene
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with
trifluoromethylaminophenyldiazir
ine)

=>